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Literature Review for EXPLORE-I A River Basin Water Quality Model Appendix A

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APPENDIX A

LITERATURE REVIEW

for

EXPLORE-I: A RIVER BASIN WATER QUALITY MODEL

by

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The Appendix to "EXPLORE-I: A River Basin Water Quality Model" contains a comprehensive review of various water quality submodels, river and estuary hydrodynamic models, and deep reservoir hydrothermal models.

The water quality submodels identified in this work are the result of an extensive literature survey of over three hundred seventy published articles and books.

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SUMMARY

This Appendix to "EXPLORE-I: A River Basin Water Quality Model" contains a comprehensive review of various water quality submodels, river and estuary hydrodynamic models, and deep reservoir hydrothermal models.

The water quality submodels identified in this work are the result of an extensive literature survey of over three hundred seventy published articles and books. The primary water quality submodels reviewed were:

- Biochemical Oxygen Demand (BOD)
- Benthic BOD
- Total Organic Carbon
- Dissolved Oxygen
- Nitrogen
- Phosphorus
- Algae
- Toxic Compounds

A complete list of the literature reviewed is contained in the bibliography at the end of this Appendix.

A number of hydrodynamic models were reviewed to identify a computer model capable of simulating various hydraulic regimes: open channel flow, tidal flow, and stratified flow.

Several deep reservoir hydrothermal models were identified and reviewed.

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SECTION A-1

QUALITY MODEL LITERATURE REVIEW

BIOCHEMICAL OXYGEN DEMAND

Biochemical oxygen demand (BOD) is a measure of the amount of oxygen required by microorganisms to decompose aerobically the organic material present in a sample under specific laboratory conditions. Although the BOD is a measure of the oxygen demand, it has long been used as a measure of the concentration of biologically decomposable organic matter present.

The BOD of a waste depends in a very complicated manner on the composition of the waste, the types of microorganisms present, and various physical factors. In general the BOD has been observed to occur in two stages, the carbonaceous stage in which heterotrophic organisms oxidize the carbonaceous fraction of organic material and the nitrogenous stage in which autotrophic bacteria oxidize the nitrogenous fraction of organic material. Normally oxidation of the carbonaceous material occurs much more rapidly than that of the nitrogenous material, resulting in the two-stage curve shown in Figure A-1. Courchaine[A-1] attributes the time lag observed in the nitrogenous stage to the relatively long generation time of the autotrophic bacteria (31 hours) as compared with the generation time of the heterotrophic organisms (20-30 minutes). O'Connor[A-2] states that because the carbonaceous material is normally in much larger concentrations than the nitrogenous material, its oxidation has an inhibiting effect on nitrification. In many cases the nitrogenous stage will not appear in a natural waterway because the right conditions for the growth of nitrifying bacteria cannot be maintained (Velz[A-3]).

The BOD present in natural waters is changed by physical as well as biological factors. The hydraulic pattern of the water can cause decomposable organic matter to settle out or to be scoured from deposits on the bottom. In addition, factors such as temperature, pH, and hardness can affect the type and performance of the bacteria available to oxidize the wastes. Velz[A-3] noted that these physical and chemical phenomena accounted for removal of a large fraction of the BOD in several rivers that he investigated. Both suspended and dissolved organic matter exert a carbonaceous BOD while most of the nitrogenous BOD demand is normally present in the dissolved form. Therefore, the effect of physical influences on nitrogenous BOD is slight and generally is ignored.

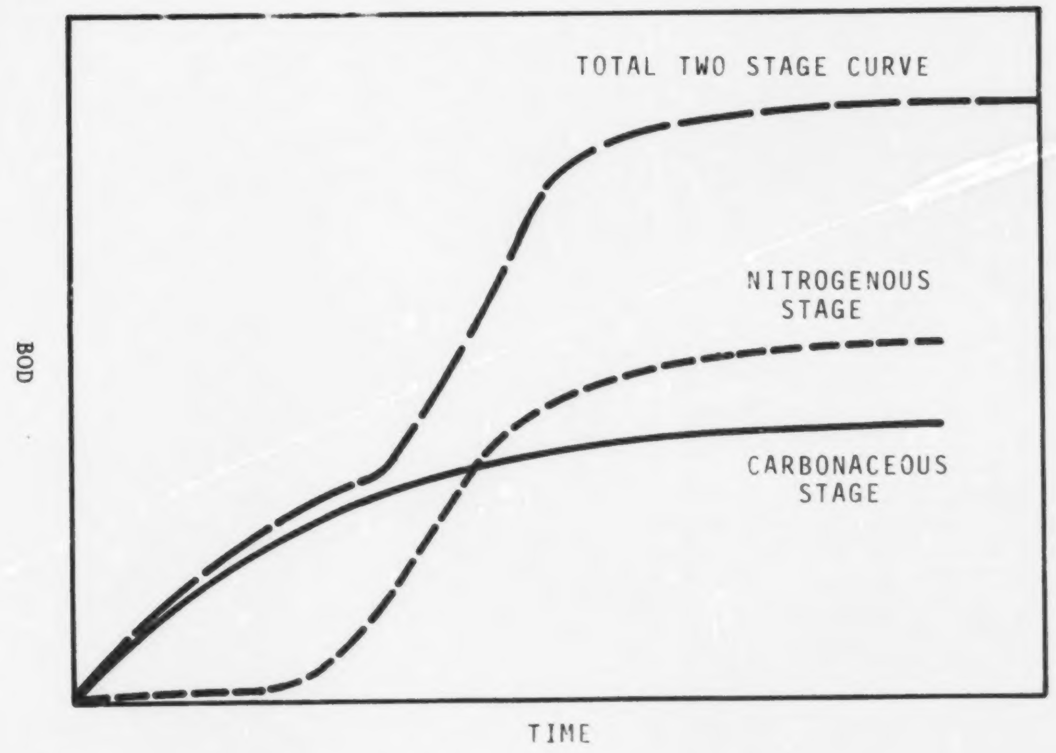

FIGURE A-1. CURVES SHOWING THE SEPARATE AND COMBINED CARBONACEOUS AND NITROGENOUS BOD STAGES AS A FUNCTION OF TIME

Review of BOD Models

The behavior of BOD in natural waters has been described for many years as a first-order reaction in which the rate of change of BOD is proportional to the amount of BOD present, or

$$\frac{dL}{dt} = -K_1L \qquad \text{(A-1)}$$

where

L = BOD at time t (mg/l)

t = time (days)

K_1 = deoxygenation coefficient (days^{-1})

It should be emphasized that this equation with K_1 as defined describes the changes in BOD due only to biological oxidation of the waste matter. The constant K_1 can be defined for a particular situation by determining the best fit of the integrated form of Equation A-1 to the available data. Numerous values of K_1 have been reported by Camp[A-4].

Additional terms have been added to Equation A-1 to account for other phenomena affecting the BOD (see Camp[A-4], O'Connor[A-5], and Dobbins[A-6]). This work has been compiled and summarized very well by Hansen and Frankel[A-7]. These authors define three separate rate constants to account for the removal of BOD in solution and suspension and another constant to account for the addition of BOD to the water due to scour of benthal deposits. Hence, the equation

$$\frac{dL_s}{dt} = -K_TL_s + P \qquad \text{(A-2)}$$

$$K_T = K_1 + K_r + K_3 \qquad \text{(A-3)}$$

where

L_s = BOD in solution and suspension

P = rate of addition of BOD to water due to physical mechanisms (scour)

K_{total} = total removal of BOD from the water due to all processes

K_1 = deoxygenation coefficient characteristic of suspended and dissolved organic matter (rate constant measured in laboratory tests)

K_r = deoxygenation coefficient due to local attached aquatic growths

K_3 = removal coefficient due to sedimentation and adsorption

Equations A-1 through A-3 satisfactorily describe only the carbonaceous stage. In order to account for the nitrogenous stage a number of authors have modified Equation A-1. For example, O'Connor[A-2] treated the carbonaceous and nitrogenous BODs as independent and governed by their own removal coefficients. The two relationships are

$$\frac{dL_c}{dt} = - K_c L_c \qquad \text{(A-4)}$$

$$\frac{dL_n}{dt} = - K_n L_n$$

where

L_c = carbonaceous BOD

L_n = nitrogenous BOD

K_c = carbonaceous removal constant

K_n = nitrogenous removal constant

Since Equations A-4 are linear, the solutions can be added together to obtain

$$L_{total} = L_c + L_n$$

The constants K_c and K_n presented by O'Connor are removal coefficients which account for all forms of loss of BOD from the system. As discussed above, K_c will not equal the deoxygenation coefficient measured in the laboratory since much of the carbonaceous material is in particulate form and can settle out. Tracor[A-8] points out that the constant K_n should closely approximate a "deoxygenation coefficient" since almost all oxidizable nitrogen is in a soluble form.

Biguria, et al.[A-9], in an analysis similar to O'Connor's, proposed that the two equations for BOD be used with a time lag between them. Their proposed equations are

$$\frac{dL_c}{dt} = -K_c L_c \quad 0 < t < t_n \tag{A-5}$$

$$\frac{dL_{total}}{dt} = -K_n L_n - K_c L_c \quad t \geq t_n \tag{A-6}$$

where t_n represents the time of onset of nitrification. The authors did not present data comparing the results of these equations with the results obtained using one first order equation.

Mathematical models other than those based on the assumption that the BOD reaction is first order have been proposed. Braun, et al.[A-10] have adopted the expressions derived by Monod which describe the relationships between bacterial growth and nutrient use rate and between bacterial growth rate and nutrient concentration. The general expression for all cases is derived by the authors, but due to the complexity of the equation a special case is considered in detail. This special case is valid for a very dilute nutrient solution defined by $K_m >> L$. The equation is

$$y = L_o - \frac{L_o + X_o/Y}{1 + \frac{X_o}{YL_o} \exp\left[\frac{\mu_{max}}{K_m}\left(\frac{X_o}{Y} + L_o\right) t\right]} \tag{A-7}$$

where

y = exerted BOD in mg/l

L_o = ultimate BOD in mg/l

t = time in days

X_o = initial microorganism concentration

Y = yield factor

μ_{max} = maximum growth rate

K_m = apparent Michaelis constant

Because of the form of this solution only three parameters need be determined: L_o, μ_{max}/K_m, and X_o/Y. These parameters were evaluated using least squares analysis to obtain a best fit to the observed data. The authors were able to obtain a better fit to data which exhibited a time lag than was possible with a first order equation. The equation will also fit data exhibiting a first order reaction; however, since only two parameters are needed to fit the first order reaction that is primarily an "over-correlation."

Young and Clark[A-11] have proposed using a second order equation of the form

$$\frac{d(L_o-L)}{dt} = K(L_o-L)^2 \qquad \text{(A-8)}$$

where K = reaction constant. Assuming K and L_o to be constant with time leads to a solution of the form

$$y = \frac{t}{\frac{1}{KL_o^2} + \frac{1}{L_o}t} \qquad \text{(A-9)}$$

The authors found that this equation fits available laboratory data with the same degree of precision as a first order reaction.

A major criticism of the first order equation is the assumption that K_1 and L_o are constant with respect to time. Dougal and Baumann[A-12] proposed a model in which K_1 and L_o were allowed to vary with time according to the relationship

$$L_o = g + \frac{t}{a+bt} \qquad \text{(A-10)}$$

$$K_1 = ct^{-d} \qquad \text{(A-11)}$$

where a,b,c,d, and g are empirically determined constants. The changes in BOD were then calculated by finite difference using the integrated form of a first order equation

$$L = L_o\left(e^{-K_1t} - e^{-K_1(t+\Delta t)}\right) \qquad \text{(A-12)}$$

where L_o and K_1 are calculated at the middle of the time interval; i.e., time = $t + \frac{\Delta t}{2}$. This model predicted observed values of BOD better, based on standard deviations of differences, than the first order equation. One drawback of this method is that five constants must be evaluated.

Dougal and Baumann also examined a second order equation similar to the one proposed by Young and Clark. This equation could be fit to their data with approximately the same accuracy as Equation A-12. However, the authors point out that neither

Equation A-12 nor the second order equation will predict long term BOD values if only the short term values are used to evaluate the constants.

Hartmann, et al.[A-13] have taken a unique approach to examine the type of equation which best describes the BOD reaction. They show that by plotting:

$$L/t \text{ versus } 1/t \ \ln\left[\frac{L_o}{L_o - L}\right]$$

for the various equations of interest [i.e., zero order, first order, second order, and the Henry equation (a combination of zero and first order reactions based on the Michaelis-Menton Equation for enzyme kinetics)] completely different loci, as shown in Figure A-2, were obtained. By plotting BOD data taken in the laboratory using meat extract and activated sludge on a similar graph, they obtained the curves shown in Figure A-3. This was interpreted as follows.

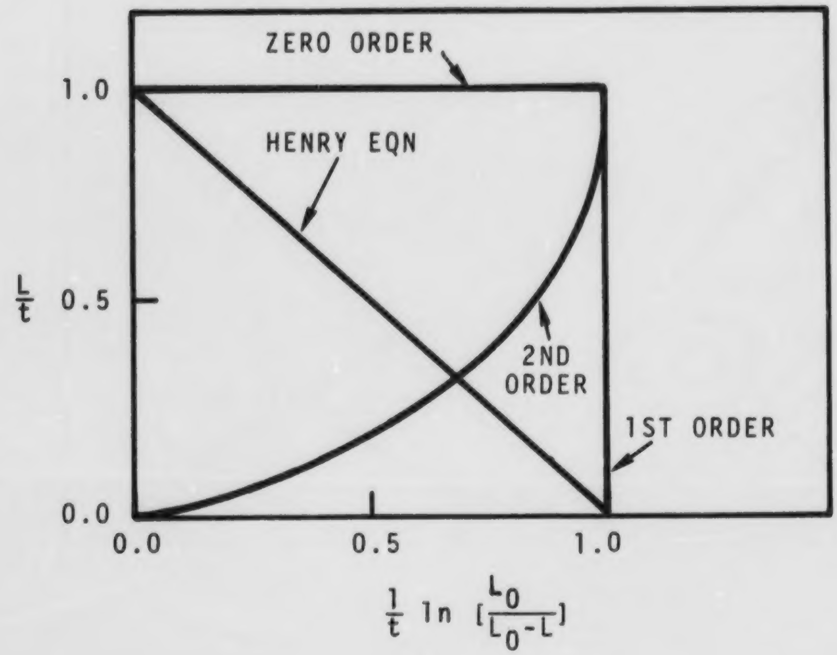

FIGURE A-2. FORM OF ZERO, FIRST, AND SECOND ORDER REACTIONS OF THE HENRY TYPE

- At low initial load values, the reaction is initially best described by the Henry Equation, which implies that the reaction is limited by the quantity of enzymes present. After reaching lower load values through biological oxidation the data follow a second order equation.
- At high initial load values the data exhibit a lag phase presumably caused by substrate inhibition. After a certain amount of decomposition the reaction follows first the Henry Equation and later the second order equation.

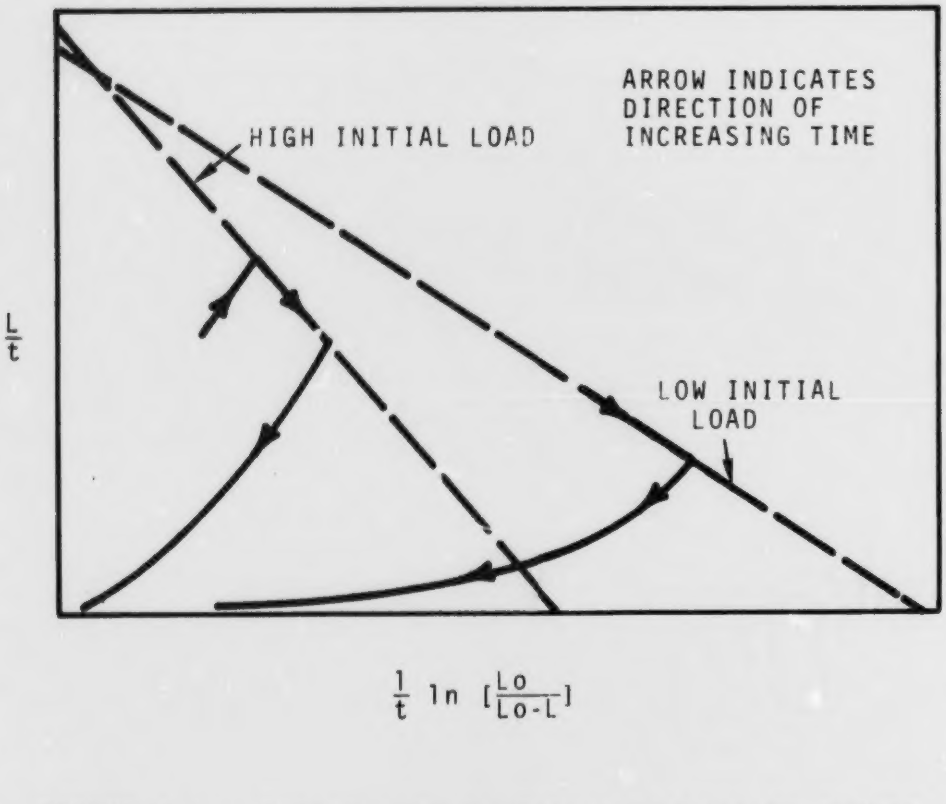

FIGURE A-3. TYPICAL BOD PLOTTED ACCORDING TO FIGURE A-2.

The authors found that in order to obtain the functional dependencies shown in Figure A-3 it was necessary to subtract the endogenous respiration of the bacteria during the entire course of the experiment. This study shows that the BOD reaction cannot be described adequately by one equation. However, one of the drawbacks to this analysis is that the endogenous respiration must be subtracted from the data before the behavior shown in Figure A-3 is obtained. When modeling the BOD in a river all of the oxygen demands are of interest. Hence, the functional dependence found by these authors is difficult to apply directly to stream modeling.

Temperature Effects on BOD

The deoxygenation race constant, K_1, has been found to vary with temperature. An empirically derived equation of the form

$$K_1 = K_1(T)\ \theta^{(T^*-T)} \qquad \text{(A-13)}$$

where

T = temperature, °C

T^* = temperature, 20°C

θ = constant

has been used in many different cases to describe this temperature dependence[A-14,A-15]. The value of the constant θ most widely used is 1.047[A-3, A-15]. Other values which have been proposed vary from 1.02 to 1.06[A-4, A-8, A-16, A-17].

Another method for describing the temperature dependence of K_1 is to assume that the BOD reaction is analogous to a chemical reaction. The Arrhenius Equation is then applicable (White, et al.[A-18]).

$$d\left(\frac{\ln K_1}{dT}\right) = -\frac{E}{RT^2} \qquad \text{(A-14)}$$

where

E = activation energy

R = gas constant

T = temperature, °K.

Integrating Equation A-14 yields

$$K_1 = A \exp\left[\left(-\frac{E}{R}\right)\left(\frac{1}{T}\right)\right] \qquad \text{(A-15)}$$

This form of the equation was used by Biguria, et al[A-9]. The constants E/R and A were evaluated separately for carbonaceous and nitrogenous BOD using treated wastewater. The data for the nitrogenous component showed that an optimum temperature was reached at 20°C and the reaction decreased for temperatures above or below this value. Hence, two equations of the form shown in Equation A-15 were necessary to describe this effect.

If Equation A-14 is evaluated as a definite integral with the limits K_1^* and K_1 and T^* and T, the following equation is obtained:

$$K_1 = K_1^* \exp\left[\left(-\frac{E}{R}\right)\frac{T - T^*}{TT^*}\right] \qquad \text{(A-16)}$$

Camp[A-4] indicates that this equation yields values in the same range as the empirically derived Equation A-13.

Camp[A-4] references experiments which indicate that the ultimate first stage BOD is a function of temperature. Values of 1 - 3% increase in the ultimate BOD with each degree C increase in temperature (and a corresponding decrease with decreasing temperature) are quoted. Biguria, et al.[A-9] reported no change of ultimate BOD with temperature over a range of 10 to 30°C.

Stoltenberg and Sobel[A-19] felt that the above formulations were not applicable over a wide range of temperature values. Instead they determine a quadratic estimate for K_1,

$$K_1 = 0.090569 - 0.009416T + 0.000879T^2 \qquad \text{(A-17)}$$

where T = temperature in °C. This equation was obtained by statistical correlation of data taken for the Delaware Estuary.

BENTHIC BIOCHEMICAL OXYGEN DEMAND

The oxygen demand of the benthic layer can be considered as composed of two separate parts, the demand of the organic sludge undergoing decomposition on the bottom of the waterway and the photosynthetic and respiratory contributions of attached algae and rooted aquatic plants. This section will consider the oxygen demand of the organic sludge. The photosynthesis and respiration of attached algae and rooted aquatic plants will be discussed later.

Camp[A-4] has proposed that the oxygen demand of bottom deposits due to sludge decay be described by a first order equation

$$L_d = L_{do}\ 10^{-K_4 t} \qquad \text{(A-18)}$$

where

L_d = biological oxygen demand per unit area of benthos

L_{do} = biological oxygen demand per unit area at time $t = 0$

t = time

K_4 = rate constant

Equation A-18 assumes that additional sludge is not added to the initial mass. Values for K_4 are reported by Camp to be between 0.0027 and 0.0033.

Velz[A-3] developed a similar equation but included the deposition of new material

$$S = \frac{D}{2.3\ K_4}\left(1 - 10^{-K_4 t}\right) \qquad \text{(A-19)}$$

where

S = cumulative storage of BOD load

D = rate of deposition of BOD

K_4 = rate constant

t = time

The author recommends a value of K_4 (base ten) of 0.03. The steady state value of the BOD load can then be found by allowing $t \rightarrow \infty$ to obtain

$$S = \frac{D}{2.3K_4} \tag{A-20}$$

If the author's value of $K_4 = 0.03$ is used then the equilibrium value of S per unit of BOD deposited is about 14.5 times the daily load deposited.

Hansen and Frankel[A-7] have stated that the benthic oxygen demand consists of two distinct parts, the BOD added to the supernatant water by physical reentrainment of organic matter and the demand of the anaerobic decomposition products which diffuse to the surface of the sludge. They propose the equation

$$\frac{1}{H}\frac{dL_d}{dt} = -K_4\frac{L_d}{H} - P \tag{A-21}$$

which when integrated becomes

$$\frac{L_d}{H} = \left[\frac{L_{do}}{H} + \frac{P}{K_4}\right]e^{-K_4 t} - \frac{P}{K_4} \tag{A-22}$$

where

L_d = areal BOD of the benthos

K_4 = rate constant for the anaerobic fermentation process

H = depth

P = rate of physical entrainment

The first term on the right side of Equation A-22 describes the demand of the anaerobic decay products and the second term accounts for the reentrainment of oxygen demanding material in the overlying water. Where sedimentation rather than scouring is occurring (P = 0) and equilibrium conditions (where the BOD exerted and that deposited are equal) have been obtained, the benthic BOD is given by

$$L_d = \frac{K_3}{K_4} HL_s \tag{A-23}$$

where the variables are as previously defined.

Ogunrombi and Dobbins[A-20] determined from laboratory experiments that in general the demand of the reentrained material is about 28 percent of the demand of the anaerobic decomposition products.

Oldaker, et al.[A-21] used Camp's equation and examined the effect of various parameters on the constant K_4. The authors studied bottom sediments from the Merrimack River in Massachusetts and found that K_4 was a function of the age and depth of the deposit. The "recent" material had a higher fraction of organic matter than the "aged" material, and the constant K_4 was higher for recent material than for aged material. The constant K_4 also increased as the depth of the benthal layer increased between 1.5 cm and 15 cm, but did not change when the layer depth increased beyond 15 cm.

Edwards, et al.[A-22] found no variation in the rate of oxygen consumption with mud depth between 4 cm and 17 cm. The rate of oxygen consumption was found to be proportional to the oxygen concentration in the overlying water according to the expression

$$y = a\,C^{b} \qquad \text{(A-24)}$$

where

y = oxygen consumption of mud

C = oxygen concentration in overlying water

a,b = constants

The best value of b was found to be 0.45 for most muds not containing midge larvae.

McDonnell, et al.[A-23] note that investigations have shown that microbial respiration is independent of oxygen concentration while respiration of algae, aquatic macrophytes and microinvertebrates is dependent on oxygen concentration. Based on this they proposed a two-part equation, one term a constant and one term dependent upon the oxygen concentration:

$$U_d = U_c + U_I\,(1 - e^{-KC}) \qquad \text{(A-25)}$$

where

U_d = total observed oxygen uptake rate

U_c = constant oxygen uptake rate

U_I = maximum variable uptake rate

C = oxygen concentration

K = rate constant

The authors determined, using benthal material from a highly eutrophic stream, that U_c was 45-48 percent of U_d and U_I was 52-55 percent of U_d.

A review by McDonnell and Hall[A-23] of the effects of temperature on oxygen consumption states that the temperature variation of the oxygen uptake rate can be described as

$$U_1 = U_2 \, e^{Kt} \tag{A-26}$$

with K varying between 0.065 and 0.077. Tracor[A-8] assumed that the benthic uptake was given by

$$U_t = 2.0 \, e^{0.07(T-20)} \tag{A-27}$$

TOTAL ORGANIC CARBON

The majority of articles published concerning total organic carbon (TOC) have been directed toward determining a general relationship between TOC data and BOD or COD data (for example, see Ford, et al.[A-24]). Two problems have been encountered in attempting to correlate the results of these data. First, the ratios of TOC/BOD and TOC/COD change from one type of waste to another. Jones[A-25] attributes this variation to the fact that while the TOC test measures the amount of organic carbon present, it yields no information about the chemical form of the carbon or its ability to be degraded biologically. Hence, no information is given as to the fate of the organic carbon in an aqueous system. Second, according to data presented by Ford[A-26] the ratios of TOC/BOD and TOC/COD change as the waste undergoes oxidation so that ratios determined at one point in time would not be the same at a later time.

Busch[A-27] has pointed out that while knowledge of TOC/BOD or TOC/COD ratios can be useful for specific problems, there is a more basic use for TOC measurements. In water where only soluble organics are significant, TOC measurements taken in conjunction with the COD test can reveal the total amount of carbon in the sample that is available to bacteria for cell synthesis. This can then be related to the oxygen demand in a stream by assuming an oxygen equivalent for the bacterial cells.

Proposed Model for Total Organic Carbon

Since no models for describing the fate of TOC in a waterway were found in the literature the following method is proposed. Organic carbon can generally be classed into one of two groups: carbon that is part of a compound which will be degraded biologically and carbon that is refractory with respect to biological decomposition. If it is assumed that the reactions of TOC can be described by a first order equation in a manner analogous to the processes affecting BOD, the following equation can be written.

$$\frac{\partial C_T}{\partial t} = -(M_1 + M_3)\, C_B - M_3\, C_R + P_B + P_R \qquad \text{(A-28)}$$

where

C_T = concentration of total organic carbon

C_B = concentration of organic carbon which is biologically degradable

C_R = concentration of organic carbon which is refractory with respect to biological degradation

M_1 = rate constant for removal of TOC due to biological oxidation

M_3 = rate constant for removal of TOC due to sedimentation and sorption

P_B = scour of biologically degradable organic carbon

P_R = scour of refractory organic carbon

$$C_T = C_B + C_R \qquad \text{(A-29)}$$

One difficulty in using Equation A-28 is that values of C_B and C_R have not been determined for most cases. The following analysis will relate these variables to parameters that have been measured. The chemical oxygen demand (COD) of a sample can be given as

$$D_T = D_R + D_B + \sigma \tag{A-30}$$

where

D_T = COD of sample

D_R = COD of refractory carbon in sample

D_B = COD of biologically degradable carbon in sample

σ = COD of other material in the sample

Assuming that σ is negligible and that D_B is the same as the BOD of the sample,

$$D_R = D_T - L_c \tag{A-31}$$

where

L_c = BOD of the carbonaceous component of the sample.

If it is further assumed that the oxygen demands of D_R and L_c are directly proportional to the carbon concentrations C_R and C_B, respectively, then

$$\begin{aligned} C_R &= A_R\, D_R \\ C_B &= A_B\, L_c \end{aligned} \tag{A-32}$$

where

A_R = proportionality constant for refractory organic carbon

A_B = proportionality constant for biologically degradable organic carbon

Combining equations A-29 and A-32 gives

$$C_T = A_B\, L_c + A_R\, D_R \tag{A-33}$$

or, from Equation A-31,

$$C_T = (A_B - A_R)\, L_c + A_R\, D_T \qquad \text{(A-34)}$$

Since values of C_T, L_c and D_T have been taken for a large number of waste streams, the constants A_B and A_R can be determined by a least squares fit of Equation A-34 to the data.

Eliminating C_R by combining Equations A-29 and A-28 and replacing C_B with Equation A-32 in Equation A-28 gives

$$\frac{\partial C_T}{\partial t} = - M_1\, A_B\, L_c - M_3\, C_T + P_B + P_R \qquad \text{(A-35)}$$

It should be noted that Equation A-35 can be derived without the use of Equations A-30 through A-34 if it is assumed that C_B is proportional to L_c. However, it is felt that by using Equation A-34 to determine the constant A_B a better correlation may be possible. Because the biologically degradable organic carbon was assumed to be proportional to the BOD (Equation A-32) it can also be assumed that the rate constants M_1 and M_3 will correspond to the rate constants for BOD degradation, K_1 and K_3.

DISSOLVED OXYGEN

Dissolved oxygen (DO) concentrations in a stream are influenced by a variety of interrelated factors. Dobbins[A-6] and Hansen and Frankel[A-7] have summarized the factors which may contribute to a change in DO concentrations. The most important ones are

- bacterial oxidation of organic matter (deoxygenation),
- reaeration,
- algal and plant photosynthesis and respiration,
- benthal demand, and
- temperature.

The first four categories represent more or less independent phenomena, all of which are influenced by temperature. The BOD and benthic demand models and the influence of temperature on them have been discussed. This section will discuss the phenomena of reaeration.

The Dissolved Oxygen Equation

The reaeration of well-mixed pure water is proportional to the oxygen saturation deficit[A-28]. Mathematically this can be expressed as

$$\frac{dD}{dt} = + K_2 D \tag{A-36}$$

where

$D = C_s - C$ = dissolved oxygen deficit

C = dissolved oxygen concentration

C_s = saturated dissolved oxygen concentration

K_2 = reaeration coefficient

The value of C_s for natural, unpolluted streams can be calculated from the equation [A-29].

$$C_s = 14.652 - 0.41022T + 0.0079910T^2 - 0.000077774T^3 \tag{A-37}$$

where T = temperature, °C.

The general equation for dissolved oxygen consists of a mass balance on the oxygen sources and sinks mentioned above, as follows:

$$\frac{dD}{dt} = + (K_1 + K_r)\ L_s + K_4 \frac{L_d}{H} - K_2 D - (P\text{-}R)_{phyto} - (P\text{-}R)_{ben} \tag{A-38}$$

where $(P\text{-}R)_{phyto}$ and $(P\text{-}R)_{ben}$ refer to the photosynthesis and respiration contributions of phytoplankton and benthic plants, respectively, and the other terms are as defined previously.

Review of Models for Reaeration Coefficient

Most attempts at defining the reaeration coefficient, K_2, in streams have been based on the assumption that K_2 is proportional to some function of turbulence or surface renewal [f(v)] divided by some function of stream depth [g(h)]; i.e.,

$$K_2 \ \alpha \ \frac{f(r)}{g(h)} \tag{A-39}$$

Numerous forms of f and g have been proposed, but $f \ \alpha \ u^n$ and $g \ \alpha \ h^m$, where u is the velocity, h is the average depth, and n and m are empirically determined exponents have been used widely.

O'Connor and Dobbins[A-30] proposed one of the early models for reaeration which was based on measurable variables rather than empirical correlations. They applied the principles of turbulent flow and derived the expressions

$$K_2 = 480 \frac{D_m^{1/2} S^{1/4}}{h^{5/4}} \quad \text{Nonisotropic turbulence} \qquad (A\text{-}40)$$

$$K_2 = \frac{(D_m u)^{1/2}}{2.31\ h^{3/2}} \quad \text{Isotropic turbulence} \qquad (A\text{-}41)$$

where

D_m = liquid film diffusion coefficient

S = slope of river channel

h = average depth of liquid

u = velocity

The distinction between isotropic and nonisotropic turbulence was based on the Chezy coefficient, $C = \frac{u}{\sqrt{hs}}$. For values of C less than 17 (or channel depths less than 5 ft if C could not be determined) the flow was considered to be nonisotropic; for all other cases flow was considered to be isotropic.

More recently Dobbins[A-6] combined theories on gas transfer to develop the following equation for K_2.

$$K_2 = \frac{0.12\ C_A A E^{3/8} \coth\left(\frac{BE^{1/8}}{C_4^{1/2}}\right)}{C_4^{3/2}\ h} \qquad (A\text{-}42)$$

where

$$C_4 = 0.9 + \frac{u}{\sqrt{gh}}$$

$$C_A = 1.0 + \left(\frac{u}{\sqrt{gh}}\right)^2$$

$$A = 9.68 + 0.054\ (T-20)$$

$B = 0.976 + 0.0137\ (30-T)^{3/2}$

$E = 30\ Su$

u = velocity

g = gravitational constant

h = depth of liquid

S = slope of channel

T = temperature

In deriving Equations A-40 through A-42 the authors assumed that the surface renewal rate equaled the velocity gradient at the surface. This assumption has been questioned by a number of other authors[A-28, A-31, A-32].

Churchill, et al.[A-28] used regression analysis on extensive field data taken in unpolluted reaches of a number of Tennessee rivers and found numerous equations correlating the reaeration coefficient to different variables. The authors recommended using the equation

$$K_2 = 5.026\ \frac{u^{0.969}}{h^{1.673}} \approx \frac{5u}{h^{5/3}} \qquad \text{(A-43)}$$

Krenkel and Orlob[A-33] based their analysis of K_2 on a longitudinal mixing coefficient which accounts for the mixing caused by eddy diffusion, convection, and nonuniform velocities. Their equation is

$$K_2 = 1.138 \times 10^{-5}\ \frac{{D_L}^{1.321}}{h^{2.32}} \qquad \text{(A-44)}$$

where D_L = longitudinal mixing coefficient.

Owens, et al.[A-34] took reaeration data on a number of small English streams. They found that results from Equations A-40 through A-43 did not agree very well with observed data. They found by regression analysis on their data that the equation

$$K_2 = 10.09\ \frac{u^{0.73}}{h^{1.75}} \qquad \text{(A-45)}$$

fit best for fast flowing, shallow streams (0.1 ft/sec < u < 1.8 ft/sec, 0.4 ft < h < 2.4 ft). For the range of values

(0.1 ft/sec < u < 5.0 ft/sec and 0.4 ft < h ≤ 11 ft) the authors combined their data with that of Churchill[A-28] and others and recommended using the equation

$$K_2 = 9.4\ u^{0.67}/h^{1.85} \qquad \text{(A-46)}$$

Thackston and Krenkel[A-31], in an analysis similar to that of Krenkel and Orlob[A-33], found a good fit of experimental data taken on a laboratory channel with the equation

$$K_2 = 0.000015\ \frac{D_L}{h^2} \qquad \text{(A-47)}$$

The exponents of D_L and h were forced to 1.0 and 2.0 without a significant increase in the standard error of the fit. The authors point out that this equation is based on uniform two-dimensional flow and hence is not applicable to long stream reaches or short nonuniform reaches. The authors also proposed a formula which takes into account the difference between the water surface area and the actual air-water interface area. The equation, based on the Froude number, was correlated empirically with both their own data and laboratory and field data from four other authors. The equation is given as

$$K_2 = 0.000125 \left[1 + \left(\frac{u}{\sqrt{gh}}\right)^{1/2}\right] \sqrt{\frac{Sg}{h}} \qquad \text{(A-48)}$$

This equation appears to provide a better fit to a larger amount of data than do Equations A-40 through A-43. In addition, the stream velocity and depth appear only to the 1/2 power so that K_2 is not as sensitive to errors in these parameters. The authors state that the absolute lower limit of Equation A-48's applicability occurs when the turbulence is not yet fully developed. The upper limit of the equation is given as that point where white water appears and bubble entrainment becomes an important mechanism of gas transfer. This equation was developed for ideal conditions and such phenomena as the effects of surface active agents or wind were not considered.

A number of other empirical relations have been determined for various laboratory and field data. These include

Isaacs, et al.[A-35] $$K_2 = 2.833\frac{u}{h^{3/2}} \qquad \text{(A-49)}$$

Kothandaraman and Ewing[A-15] $K_2 = 5.827 \frac{u^{0.924}}{h^{1.705}}$ (A-50)

Negulescu and Rojanski[A-36] $K_2 = 4.74 \left(\frac{u}{h}\right)^{0.85}$ (A-51)

Langbein and Daram[A-37] $K_2 = 3.3 \frac{u}{h^{1.33}}$ (A-52)

Cadwallader and McDonnell[A-38] found a correlation of K_2 with the energy expenditure E, where E is assumed to be proportional to the turbulence present in the stream. The same concept was also investigated by Dobbins[A-6] and by Krenkel and Orlob[A-33]. Cadwallader proposed the equation

$$K_2 = 25.7 \frac{E^{0.5}}{h} \qquad \text{(A-53)}$$

where E = energy expenditure.

Krenkel and Orlob[A-33] found an expression of the form

$$K_2 = 1.141 \times 10^{-4} \frac{E^{0.408}}{h^{0.660}} \qquad \text{(A-54)}$$

The reaeration coefficient is a function of temperature. In general the form of the temperature dependence (Elmore and West[A-39]) has been given as

$$K_2 = K_2(20)\ \theta^{(T-20)} \qquad \text{(A-55)}$$

with values of θ ranging from 1.01 to 1.06. Elmore and West[A-39] recommended a value of 1.0241 for θ, which corresponds to an increase at a geometric rate of 2.41 percent per °C.

Thackston & Krenkel[A-31] state that the effect of wind in increasing the surface renewal rate for streams is unreliable and probably should not be used in an analysis of K_2. However, for large bodies of water such as bays and estuaries, wind velocities can have an important effect on the reaeration coefficient (Krenkel, et al.[A-16]). Juliano[A-40] observed that surface turbulence proved to be the most important factor controlling reaeration in the Sacramento-San Joaquin Delta and that wind velocity was the most significant parameter causing surface turbulence. Tracor[A-8] also noted that wind velocity had a tremendous effect on reaeration coefficients for Galveston Bay and suggested that the reaeration rate constant varies with wind velocity (w) in proportion to $\sqrt{w}$ for w greater than 10 knots.

NITROGEN

The relationships between the various forms of nitrogen present in an aqueous system are shown in Figure A-4. Elemental nitrogen can be reduced (nitrogen fixation) for use in building cells by various bacteria and blue green algae (McCarty[A-41]). Certain autotrophic bacteria will oxidize ammonia (NH_3) present in water to nitrite (NO_2-) and nitrite can be further oxidized to nitrate (NO_3-). This process, nitrification, represents the major portion of the nitrogenous component of BOD as discussed earlier. In addition, the ammonia can be directly incorporated into an organic form by either autotrophic or heterotrophic organisms. Ammonia can also escape from (or enter) the water in a gaseous form. The nitrate produced is available as a nutrient to many organisms which can convert it into an organic form. In some cases the nitrate will undergo denitrification through biological action and be converted either to nitrite or elemental nitrogen. The nitrogen in organic form can be present either as part of a living organism or as part of a nonliving organic substance (such as a soluble organic compound or part of a decaying organism). Nitrogen released from the nonliving organic substances will in general return to the water in the form of ammonia. A significant portion of the nitrogen in the organic form is refractory and will not readily return to solution or reenter the nitrogen cycle.

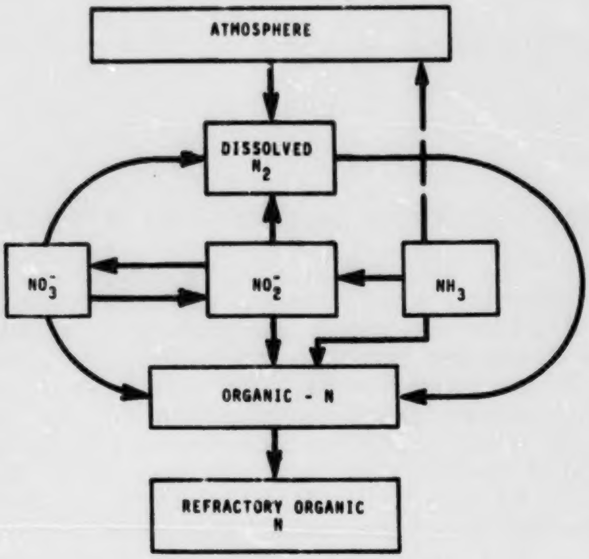

FIGURE A-4. THE NITROGEN CYCLE IN WATER AS PRESENTED BY McCARTY[A-41]

The fixation of nitrogen in Sanctuary Lake, Pennsylvania, was studied by Dugdale and Dugdale[A-42]. The results of these experiments show that for a relatively shallow fresh water lake the increase in organic nitrogen from fixation approximately equaled one percent of the total in the lake. The authors note that in the absence of other forms of nitrogen (NO_3 or NH_3) the increase may reach as high as 3 percent. But if nitrogen is abundant in its other forms, fixation will for all practical purposes cease. McCarty[A-41] points out that the elemental form of nitrogen is generally considered to be of little biological importance.

The loss of ammonia from both streams and impoundments has been studied by Stratton[A-43,A-44]. For streams the reaction was shown to obey a first order equation of the form

$$\frac{dC}{dt} = - kC \qquad \text{(A-56)}$$

where

C = concentration of ammonia nitrogen

k = rate constant

Using a small recirculating flume and synthetic river water Stratton[A-44] determined the rate constant as a function of temperature and pH to be

$$k = 0.048 \exp \{0.13 (T-20)\} \quad 15 < T < 30 \qquad \text{(A-57)}$$

$$k = 0.080 \exp \{1.57 (pH-8.5)\} \quad 7.5 < pH < 9.5 \qquad \text{(A-58)}$$

where

T = temperature in °C

pH = negative log of hydrogen ion concentration

No attempt was made by the authors to check these results on a natural stream; however, the form of the equations agreed with those presented earlier by other authors. In order to determine the ammonia loss from the surface of lakes or impoundments, Stratton[A-43] conducted two tests. In one test synthetic water was impounded in battery jars and exposed to the natural mixing of the wind, after which rate constants were calculated. A second test measured directly the ammonia gas liberated from two different lakes. The results of the direct measurements were compared with the predictions using the rate constants (corrected using Equations (A-57) and (A-58) for temperature and pH; measured values were 14% and 22% of predicted values. This discrepancy was attributed to better mixing in the battery jars, leading to rapid depletion of the dissolved ammonia. The author estimated that up to 5% of the daily ammonia input in one warm eutrophic lake studied could be lost by degasification.

The refractory organic nitrogen left in particulate form after algal decomposition has been studied by Jewell and McCarty[A-45] for aerobic conditions and by Foree and McCarty[A-46] for anaerobic conditions. The results of both studies have been summarized by Foree, et al.[A-47]. The two major controlling factors identified by these authors in the regeneration of nitrogen are the initial nutrient content of the algae and the extent of organic decomposition. The initial nutrient content is related to the nutrient concentration present when the algae culture is growing. Excess regeneration will occur when the nutrient of interest is present at concentrations far greater than necessary for optimum algae growth. In this case the nutrient is incorporated into the cell at concentrations above those required simply for growth. These "excess" nutrients are in general loosely bound in the cell and easily released when decay starts. Proportional regeneration of nutrients occurs when the concentration of the nutrient of interest is low enough to inhibit the algae growth. In this case the nutrient atoms are tightly bound in the cell and can be regenerated only when the cell is enzymatically digested. The nutrient concentration which defines the separation of excess and proportional is called the critical concentration. The extent of organic decomposition is measured by the particulate chemical oxygen demand and the ignitable suspended solids.

The authors derive the following equations which give the concentration of nitrogen held in the refractory remains of both the algae and decomposing organisms:

$$N_r = \left(\frac{f_1 f_2}{R(1-f_1 f_2)} (M_o - M_r)(f_{nd} - f_{no}) + S_r f_{no}\right) \qquad \text{(A-59)}$$

for proportional regeneration, and

$$N_r = \left(\frac{f_1 f_2}{R(1-f_1 f_2)} (M_o - M_r)(f_{nd} - f_{nc}) + S_r f_{nc}\right) \qquad \text{(A-60)}$$

for excess regeneration, where

N_r = refractory particulate nitrogen concentration

f_1, f_2, R, f_{nd} = constants evaluated from previous studies for aerobic and anaerobic cases

f_{no} = initial nitrogen content of algae

f_{nc} = critical level for nitrogen above which excess regeneration occurs

M_o = initial COD

M_r = refractory particulate COD

S_r = refractory ignitable suspended solids

These equations apply to decomposition under both aerobic and anaerobic conditions since different values of the constants f_1, f_2, R, and f_{nd} are used for the two conditions.

The experiments upon which these results are based were conducted in the laboratory under well controlled conditions varied over a wide range of values. The studies did not include such geochemical phenomena as absorption, precipitation, or entrainment which could occur in a natural waterway. To use Equations A-59 or A-60 the extent of organic decomposition (represented by M_r and S_r) must be known.

These experiments also showed that after six months to one year the decomposition process had slowed considerably. In the case of aerobic decomposition approximately 50% of the nitrogen was still in the refractory form while under anaerobic decomposition conditions approximately 60% of the nitrogen remained in the refractory form. The organic matter continued to decay past this time at a very slow rate and only a few percent per year of the refractory material were returned to the overlying water.

Foree and McCarty[A-46] have proposed a time dependent first order equation to describe the rate of decomposition of algae under dark anaerobic conditions. This equation is

$$M = (M_o - fM_o)\, e^{-kt} + fM_o \qquad \text{(A-61)}$$

where

M = particulate chemical oxygen demand concentration

M_o = initial particulate chemical oxygen demand concentration

f = refractory organic fraction

k = rate constant

t = time

The authors found a value for f of 0.40 with a standard deviation of ± 0.15 and a value for k of 0.022/day with a standard deviation of ± 0.007. In addition, the temperature dependence of the rate constant k was determined to be

$$k = k_o \exp \{C_K (T-T_o)\} \qquad \text{(A-62)}$$

where C_K has a value of 0.055/°C for the temperature range $15 < T < 25°C$.

The authors state that these results, which were determined in the laboratory for anaerobic conditions, did not differ significantly from the results of Jewell and McCarty[A-45] for decomposition under aerobic conditions.

Denitrification can be a significant sink for nitrogen under certain conditions. Brezonik and Lee[A-48] determined that approximately 11% of the total nitrogen put into Lake Mendota was removed annually through denitrification. This loss occurred during summer stratification in the hypolimnion where low dissolved oxygen concentrations existed. The rate of nitrogen loss due to denitrification was estimated to range from 8.4 mg/l/day to 26 mg/l/day. Brezonik and Lee compared these rates with those determined by other authors of 80 mg/l/day and 15 mg/l/day for widely varying environments.

In none of the articles reviewed was an attempt made by the authors to relate the denitrification process to other variables such as temperature or oxygen concentrations. In their study of the Delaware Estuary, Thomann, et al.[A-49] attributed significant nitrate losses to denitrification. However, their model did not include the denitrification process.

The process of nitrification has been studied in considerable detail because of the large oxygen demand it can exert in a body of water. Wezernak and Gannon[A-50,A-51] proposed two different equations to describe the nitrification process. In each case the equation must be written to describe each of two major components in nitrification, the oxidation of ammonia to nitrite and the oxidation of nitrite to nitrate. One of their equations is based on the Henri equation derived for enzyme kinetics and is given as

$$\frac{p}{t} = V + K \left[2.303 \log \left(\frac{S}{S_o} \right) \frac{1}{t} \right] \qquad \text{(A-63)}$$

where

p = product concentration (either nitrite or nitrate)

t = time

V, K = constants

S = substrate concentration (either ammonia or nitrite)

S_o = initial substrate concentration

The other expression is based on the Robertson autocalytic growth equation and is given as

$$\log \frac{y}{A-y} = \alpha t - a \qquad \text{(A-64)}$$

where

A = initial oxidizable substrate

y = oxidized substrate

t = time

α, a = constants

Both Equations A-63 and A-64 have two constants which are determined by best fit of observed stream data. The authors recommend using Equation A-64 because it is more accurate and easier to fit with data.

Wezernak and Gannon evaluated Equation A-64 using data taken from the Clinton River in Michigan and were able to obtain very good correlation. They have pointed out[A-52] that Equation A-64 was not meant as a strictly predictive equation and that the constants must be reevaluated whenever significant changes such as temperature, flow, or ammonia concentration occur in the stream. However, the model has the advantage that the constants can be rapidly reevaluated if conditions do change.

Stratton & McCary[A-53] have proposed using a set of equations similar to the Monod equations to predict nitrification in streams. In this case a solution is obtained by considering the substrate concentration as the variable of interest instead of the bacterial mass, as originally done by Monod. The equations are

$$-kt = \left[\frac{-K_s}{M_o + aC_o} \quad \frac{1}{a}\right] \ln \left[M_o + aC_o - aC\right] + \left[\frac{K_s}{M_o + aC_o}\right] \ln \left[\frac{CM_o}{C_o}\right] + \left[\frac{1}{a}\right] \ln M_o \qquad \text{(A-65)}$$

$$M = M_o + \int_{t=o}^{t=t} \left[\frac{aKMC}{K_s + C} - bM \right] dt \qquad \text{(A-66)}$$

$$C_{NO_2-N} = C_{NO_2-N,O} + \int_{t=o}^{t=t} \left\{ \left[\frac{kMC}{K_s + C} \right]_{NH_3-N} - \left[\frac{kMC}{K_s + C} \right]_{NO_2-N} \right\} dt \qquad \text{(A-67)}$$

where

k = substrate utilization parameter

K_s = half velocity constant (Michaels constant)

M_o = initial viable bacterial mass

C_o = initial substrate concentration

a = yield constant

b = nitrifying organism decay parameter

M = total bacterial mass

C = total substrate concentration (subscripts NO_2-N and NH_3-N refer to nitrite and ammonia nitrogen, respectively)

Equation A-65 relates time and substrate concentration as a function of the kinetic parameters. Equation A-66 yields the mass of viable organisms involved in the nitrification process. Equation A-67 gives the nitrite concentration at the end of the time interval calculated by Equation A-65. Nine parameters must be evaluated for these equations: a, k, K_s and M_o for both ammonia and nitrite oxidation and b for the entire oxidation process. The authors initially neglect the organism decay parameter and use a theoretically derived value for the two yield constants a. The other six constants are found by performing two batch tests with a sample of water. Ammonia is added to one batch and the course of the oxidation is followed.

The three constants are then determined by a best fit of the equation to the data. A similar experiment is performed to determine the constants for nitrite oxidation. The parameter b is determined by comparing substrate concentrations (predicted by using rate parameters obtained independently for ammonia and nitrite oxidation steps) with measured nitrogen concentrations. The value of b which yields the best fit is then used.

To test the validity of their prediction equations under laboratory conditions, the authors determined the rate constants from previous tests and used these constants to predict the course of nitrification for different nitrogen concentrations and different bacterial innoculation concentrations. The equations predicted the results of these tests quite well. Two limitations of the above method are pointed out by the authors. First, the rate constants must be evaluated for each particular stream under consideration rather than using an average of previously determined constants. Second, this method cannot account for any nitrification due to benthic organisms. Wezernak and Gannon[A-52] have pointed out that in some cases it is impossible to determine the appropriate rate parameters in the laboratory since the conditions found in the flowing stream cannot be duplicated accurately.

Knowles, et al.[A-54] proposed a set of equations similar to Equations A-65 - A-67 but used a different procedure for obtaining the constants and solving the equations. They report a temperature dependence of the constants (K_s) and (k) for both *nitrobacter* and *nitrosomonas*. Stratton, et al.[A-53] found a temperature dependence for the yield constant (k) but not for the Michaelis constant (K_s). They state that since the magnitude of (K_s) depends upon the measurement of the lower substrate concentration which is very difficult to measure accurately, no real conclusions about the temperature dependence of K_s can be drawn. The temperature dependence for k as reported by Stratton & McCarty[A53] is

$$\begin{aligned} &\text{Ammonia} \quad k_T = 1.47\, e^{0.084(T-20)} \\ &\text{Nitrite} \quad k_T = 4.9\, e^{0.056(T-20)} \end{aligned} \qquad \text{(A-68)}$$

where T = temperature °C.

Tracor[A-8] proposed a set of equations for predicting a nitrogen cycle based on first order reactions. The equations are based on the following scheme for decomposition of organic -N:

$$\text{Organic N} \xrightarrow{K_1} NH_3 \xrightarrow{K_2} NO_2 \xrightarrow{K_3} NO_3 \qquad \text{(A-69)}$$

Thomann, et al.[A-49] used a steady state first order kinetic model which allows both feed forward and feed back phenomena. The authors set up a series consisting of one equation for each form of nitrogen to be considered (i.e., organic, nitrite, nitrate, etc.). The coefficients of the various concentrations were determined by solving the equations to obtain a best fit to data taken from the waterway under consideration. Including advective and dispersive terms, the equations take the following forms:

$$\begin{aligned} 0 &= \nabla (E\nabla N_1) - \nabla . QN_1 - K_{11}N_1 + K_{21}N_2 + --- + K_{m1}N_m \\ 0 &= \nabla (E\nabla N_2) - \nabla . QN_2 + K_{12}N_1 - K_{22}N_2 + --- + K_{m2}N_m \\ 0 &= \nabla (E\nabla N_m) - \nabla . QN_m + K_{1m}N_1 + --- - K_{mm}N_m \end{aligned} \tag{A-70}$$

where

E = dispersion coefficient

Q = discharge

K_{ij} = reaction coefficient

N_i = concentration of i^{th} form of nitrogen

These equations can be formulated into a matrix equation which can be solved by standard matrix inversion techniques. The authors used this model to predict the concentration of various forms of nitrogen in the Potomac and Delaware Estuaries with reasonable accuracy. However, the authors note that the rate coefficients used do not represent a unique set of constants since they were determined for the particular conditions present at the time the data were taken. In some cases different rate constants were used for different stretches of river. For example, in a 15-mile stretch of the Delaware Estuary a greatly reduced nitrification rate constant was required to match the high ammonia concentration present. It was hypothesized that the nitrification process was inhibited along this reach by extremely low dissolved oxygen concentrations.

PHOSPHORUS

The phosphorus cycle in an aqueous system is shown in Figure A-5. Inorganic phosphorus is most commonly present in minerals or dissolved in water as orthophosphate (PO_4). Particulate inorganic phosphates are in general only slightly soluble in water and are not used by aquatic life. Complex or condensed phosphates are unstable in water and will hydrolyze slowly to orthophosphate. Plants and other aquatic organisms can assimilate either dissolved orthophosphate or soluble organic

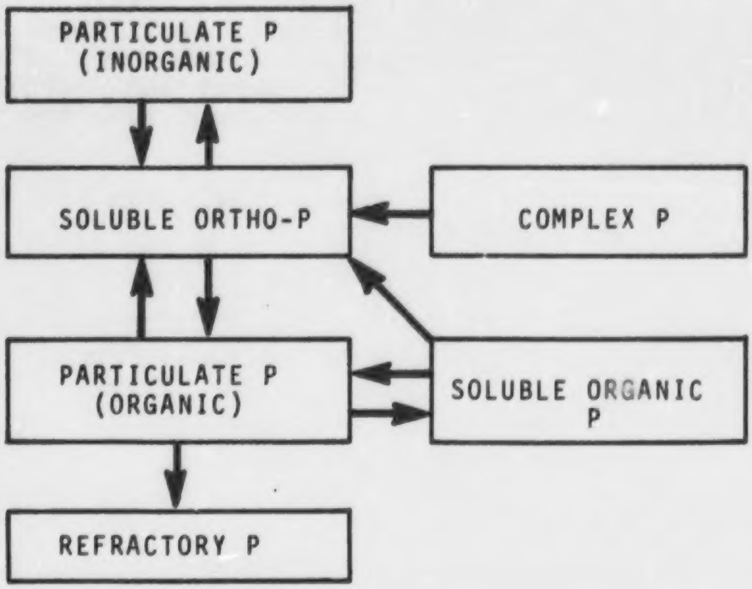

FIGURE A-5. THE PHOSPHORUS CYCLE IN WATER AS PRESENTED BY McCARTY[A-41]

phosphate. The biota will excrete either soluble organic phosphate or orthophosphate during both growth and death. If the soluble organic phosphate is not reassimilated it will hydrolyze to orthophosphate. Upon death of the aquatic organisms, a certain fraction of the phosphorus in the cells is retained in a refractory state.

The reaction rates and concentrations of phosphorus are not generally well known for two reasons. First, it is difficult experimentally to determine phosphorus levels with acceptable accuracy[A-41,A-55]. Second, the reactions are complicated by many physical variables and must include both chemical and biological effects[A-56].

The interactions of phosphorus between the sediments and the overlying water have been studied by Stumm and Lecke[A-57] who concluded that for an undisturbed sediment-water interface, the maximum contribution of phosphorus the sediments can make to the overlying water is approximately 9×10^{-6} moles/M^2/day.

The hydrolysis of condensed phosphates has been reviewed by Heinke and Norman[A-56]. They indicate that the rate of hydrolysis is affected as shown in Table A-1.

TABLE A-1. FACTORS WHICH INFLUENCE RATE OF HYDROLYSIS

Variable	Functional variation of rate of hydrolysis
Temperature	Given by Arrhenius equation
pH	Logarithmic dependence
Enzymes (organisms)	Presence can increase rate up to 10^6 times
Concentration	First order equation

The authors note that there is insufficient evidence available to determine the quantitative dependence of the rate of hydrolysis on the concentration or types of organisms present. Rate constants for "natural waters" are reported in the range of 7×10^{-4} to 2×10^{-3} mg PO_4/l min and for "wastewater" in the range 10^{-3} to 2×10^{-2} mg PO_4/l min.

Keup[A-58] studied the assimilation of phosphorus in two rivers which were very different ecologically. In both cases he determined that the phosphorus assimilation could be described by a first order reaction. The author states that the primary mechanism of phosphorus uptake is the stream biota but that the ultimate removal of the phosphorus from the waterway is related to the physical nature of the waterway. The phosphorus is stored in refractory organic and mineral form in the bottom sediments. These sediments are scoured during periods of high flow and the phosphorus is washed out of the waterway. Keup found the rate constant for the South Platte River in Colorado, a clean sandy bottomed stream containing mostly attached algae, to be 0.011 per mile. The Pigeon River in North Carolina, a mountain stream with considerable pollution, had a rate constant of 0.02 per mile.

Tracor[A-8] has proposed a model for phosphorus based on the scheme shown in Figure A-6. The equations describing the dynamics for this scheme are

$$\frac{da}{dt} = W - K_1 a + K_3 c$$

$$\frac{db}{dt} = K_1a - K_2b + K_4c \qquad \text{(A-71)}$$

$$\frac{dc}{dt} = K_2b - K_3c - K_4c$$

where

a = inorganic phosphorus concentration (mg/l)

b = concentration of phosphorus in protoplasm (mg/l)

c = soluble organic phosphorus concentration (mg/l)

W = phosphorus source (mg/l/day)

k_1, k_2, k_3, k_4 = rate constants (1/day)

The authors give no indication as to how the rate constants are to be evaluated.

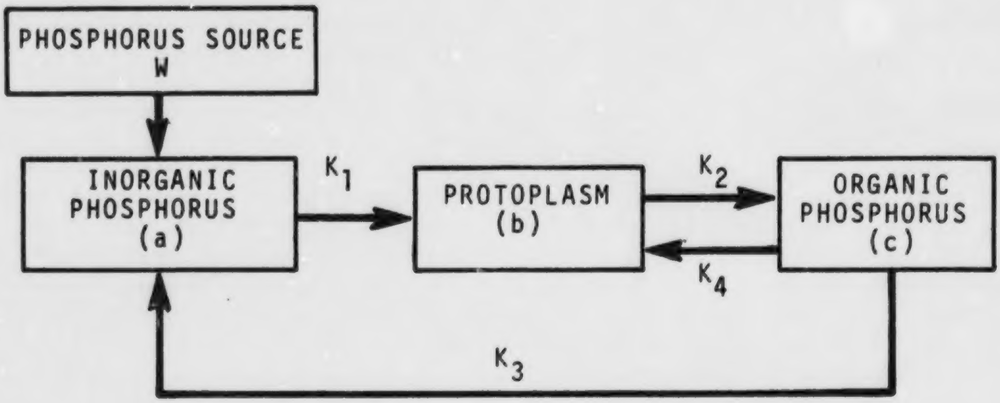
PHOSPHORUS SOURCE
W
INORGANIC
PHOSPHORUS
(a)
K1
PROTOPLASM
(b)
K2
K4
ORGANIC
PHOSPHORUS
(c)
K3

FIGURE A-6. SCHEMATIC FOR MATHEMATICAL MODEL FOR PHOSPHORUS PROPOSED BY TRACOR[A-8]

A method of calculating the fractions of refractory phosphorus in decaying algae has been presented by Foree, et al.[A-47]. The method is identical to that used for calculating refractory nitrogen. This method was covered in detail in the discussion of nitrogen.

ALGAE AND ATTACHED PLANTS

The modeling of algae is inherently complex because of the heterogeneous algal population and the myriad of interacting environmental factors which influence algal dynamics. For example, algae growth rates are complex functions of a large number of environmental parameters such as temperature, pH, macro-nutrient concentrations, irradiance, and the presence of trace minerals. In addition, the effects of these parameters on the algae growth rates vary widely from one type of algae to another. Algae are also part of a complicated food web which is difficult in itself to model.

Algae have been separated into two categories, (1) planktonic (unattached) algae and (2) sessile (attached) algae. Sessile algae, attached plants, and other micro- and macroorganisms that reside on the bottom of the water course have been collectively classified as benthic organisms.

Most algae modeling efforts have been directed toward describing their influence on the dissolved oxygen concentration in the river course rather than toward modeling the algal concentrations per se. In evaluating the water quality models associated with algae, three separate areas will be reviewed: phytoplankton photosynthesis and respiration (P-R), benthic P-R, and planktonic algae concentrations.

Photosynthesis and Respiration

The effect of algal photosynthesis and respiration (P-R) on the dissolved oxygen (DO) concentrations in natural waters can be quite important. In many cases photosynthesis can provide as much as two-thirds of the dissolved oxygen present in the water (Camp[A-4]). At the same time the nighttime respiration of the algae may deplete the oxygen resources of a river. The mathematical modeling of photosynthesis and respiration has generally been handled in one of three ways. First, the mean (usually daily) gross or mean net oxygen production is determined in terms of environmental parameters and is considered to be a constant when used in a DO model. Secondly, the oxygen production is modeled as a function of time and the equations are fit to experimental data to account for the diurnal variations in DO due to photosynthesis and respiration. Once the diurnal variation is obtained it is assumed to be constant from day to day. Third, the P-R are related to the concentration of phytoplankton present in the water.

A model of the first type has been used by Camp[A-59] and by Dobbins[A-6]. The mean daily net contribution of photosynthesis and respiration to DO is considered to be a constant α. Dobbins evaluated α by determining values for all other parameters in his dissolved oxygen equation and then using the value of α that gave the best fit of the equation to the experimentally measured DO levels. Camp evaluated the constant α using the experimental light and dark bottle techniques. In both cases the authors were able to fit the DO profile measured in the stream with their equations. One difficulty with this method of modeling is that it is very easy to lump a number of variables together in one constant so that the constant does not actually represent the parameters of interest.

Hansen and Frankel[A-7] have pointed out two shortcomings of this method. First, as the time period becomes large the DO concentration becomes a constant. Hence, one must be careful to use the equation only over short time periods. Second, for a very small reaeration coefficient the DO concentration is independent of the P-R levels. However in an impoundment, for example, reaeration may be insignificant and P-R could be a major source of oxygen.

To incorporate the effects of temperature on the mean rate of P-R, Davidson and Bradshaw[A-60] used a parabolic temperature factor based on data from McCombie[A-61]. They then assumed that the average daily photosynthesis, P, is given by $\frac{P_{max}}{\pi}$ (i.e., photosynthesis is described by a half sine wave) and that the respiration, R, can be given by $P = \beta R$ so that the daily net contribution of P&R to DO is given by

$$\overline{P-R} = \frac{\beta-\pi}{\pi(\beta-1)} \quad 25-0.028\ (T-303)^2 \qquad \text{(A-72)}$$

where

$\overline{P-R}$ = mean daily net DO produced

β = constant of proportionality between P and R

T = temperature, °K

The constant β is adjusted to yield the desired average value of $\overline{P-R}$. The authors stated that in general β had a value between 1 and 10 but did not elaborate on the adequacy of this expression in describing the P&R of algae.

Doudoroff, et al. (see References A-62 and A-63) have found that the minimum dissolved oxygen concentration rather than the mean value is important to fish life. Hence, in many cases it is important to predict the DO contribution by P-R on an hourly basis. Biguria, et al.[A-9] proposed an equation of the form

$$P\text{-}R = C \left\{ \exp \left\{ \left[\frac{E}{T+273} \right] \right\} \right\} \left\{ \sin \left[\frac{\pi t}{12} \right] \right\}^{n} \qquad \text{(A-73)}$$

and fitted data by regression analysis to determine the constants C and n. The authors reported that good correlation could be obtained within the temperature range of the data (15-22°C), but outside that range the results were unacceptable.

Another method, first presented by Odum and used by O'Connor and DiToro,[A-64] is to assume that the photosynthetic rate is directly proportional to the sunlight intensity which varies as a half sine wave. The rate of photosynthesis can then be expressed as a Fourier series

$$P(t) = P_m \left\{ \frac{2tp}{\pi} + 2 \sum_{n=1}^{\infty} a_n \cos \left[2\pi n (t - tp/2) \right] \right\} \qquad \text{(A-74)}$$

where

$P(t)$ = photosynthetic rate

P_m = maximum photosynthetic rate

tp = time period under consideration

t = time

$$a_n = \frac{2\pi/tp}{\left(\frac{\pi}{tp}\right)^2 - (2n\pi)^2} \cos(n\pi tp).$$

The respiration rate is considered to be a constant. This model was incorporated into an equation for DO and fitted to diurnal DO data taken from the Grand River in Michigan. The equation agreed very closely with the data for a number of cases. The authors did not state in the article whether the constants in Equation A-74 were refitted to each set of data shown or determined once and then not changed.

Using a similar analysis, Kartchner, et al.[A-62] found that the first two terms of a Fourier expression could be used to describe the DO variation for a single diurnal cycle. The purpose of using the Fourier series was not to model the DO contributions of P-R but to provide a method of analysis of DO for comparison of the data. Hence, in each set of data the constants in the series were reevaluated to give a best fit.

Hansen and Frankel[A-7] propose using a single term periodic function to describe the P-R contributions

$$P\text{-}R = a \cos(wt + \phi) \qquad \text{(A-75)}$$

where

$P\text{-}R$ = net rate of DO produced at time t

a, ϕ = constants

w = period of cycle (daily)

This model was included in a DO model and tested on the Flint River in Michigan. The constants in the equation were adjusted to make the calculated and measured minimum DO levels coincide. The model predicted the maximum DO level quite well and in general followed the trends of the DO curve.

Biguria, et al.[A-9] proposed an equation to relate net oxygen production to temperature and time of the form

$$P\text{-}R = g_1 + g_2\,(T+273)^{-1} + \sum_{n=1}^{2} \left\{ a_n \sin\left(\frac{n\pi t}{12}\right) + b_n \cos\left(\frac{n\pi t}{12}\right) \right\} \qquad \text{(A-76)}$$

where the six constants would be determined by regression analysis. However, this model was rejected by the authors because of the difficulty in using the equation.

None of the models discussed above relate the P-R rates to the concentration of phytoplankton actually measured in the water. Bain[A-65], using data from a number of other authors, related the P-R rates to the concentration of algae measured in terms of chlorophyll concentrations.

$$P_{max} = 0.010\,\alpha \qquad \text{(A-77)}$$

$$R = 0.001\,\alpha$$

where

P_{max} = maximum photosynthetic rate at surface, mg/l/hr

R = maximum respiration rate, mg/l/hr

α = cholorophyll concentration, mg/l

A linear correction to P_{max} was then made to account for light attenutation in the euphotic zone. A temperature correction was applied to R (but not to P_{max}) based upon the reaction doubling with each 10°C increase in temperature. A dissolved oxygen model using the P-R model was applied to the San Joaquin River near Mossdale and predicted the DO concentrations reasonably well.

In experiments on the Sacramento-San Joaquin estuary, Bailey[A-66] correlated the daily mean gross photosynthesis to a number of factors with the equation

$$P = 3.16\ C_h \frac{I^{2/3}}{k_e} + 0.16\ T - 0.56\ H \qquad \text{(A-78)}$$

where

P = mean gross photosynthesis

C_h = mean chlorophyll concentration

I = mean daily solar intensity

k_e = light extinction coefficient

T = mean temperature

H = mean water depth

Correlation using this method was quite good; however, Bailey noted the inability of present techniques to adequately predict chlorophyll concentrations under changing environmental conditions. Biguria, et al.[A-9] noted that data in the literature were insufficient to permit regression on the equation.

Benthal Oxygen Demand

The oxygen demand of the benthic layer can be considered to have two separate parts, the photosynthetic and respiratory contributions of attached algae and rooted aquatic plants and the demand of the organic sludge undergoing decomposition on the bottom of the waterway. The dissolved oxygen contributions due to photosynthesis and respiration of attached algae and rooted aquatic plants can be treated in a manner analogous to phytoplankton. O'Connell and Thomas[A-63] measured the net effect of P-R on the DO levels in the Truckee River where benthic algae were abundant and little or no phytoplankton were present. These authors found that, in general, respiration of the benthic plants exerts a greater strain on the oxygen resources of the river than do phytoplankton, because the nighttime respiratory demand is more localized along the length of the stream and the demand is placed on a body of water that does not have the advantage of receiving the additional oxygen from photosynthesis during the daytime.

Planktonic Algae

A number of early attempts to model plankton in the marine environment have been reviewed by Riley[A-67]. These models are based on relationships similar in form to Volterra's equations describing, in an idealized manner, the prey-predator relationship. Each consecutive model introduces an additional degree of complexity to better simulate observed algal behavior. The six physical and environmental factors found by these early models to have significant influence on the phytoplankton populations are listed by Riley as:

Irradiance - I
Depth - Z
Nutrients - N
Temperature - T
Predators - H
Vertical Turbulence - V

Smith[A-68] has approached the modeling of algae by looking at their position in the food web. He used a systems analysis treatment based on population dynamics. According to Smith, the form of the model is as important in predicting population trends as the magnitudes of the various parameters used in the model. For example, suppose that the study of a system composed of three trophic levels yields certain stable densities at each level and shows how these densities change in relation to each other and with time. If a fourth trophic level is added to this system the stable densities of the levels and the dynamics relating the levels will be very different, even if the magnitudes of the parameters used are the same.

Smith proposes a general model based on the algebra of enzyme kinetics for three trophic levels. The equations are derived by taking a mass balance for each trophic level based upon the reaction

$$F + A \xrightarrow{x} B \xrightarrow{y} 2A \qquad \text{(A-79)}$$

where for the particular trophic level under consideration

F = food density

A = density of feeding population

B = density of anabolizing portion of population

x, y = rate constants

$N = A + 2B$ = total population

A constant total density for the system is assumed:

$$S = R + N_1 + N_2 + N_3 = \text{Constant} \qquad \text{(A-80)}$$

where

S = total density

R = free resonances

N_1, N_2, N_3 = total population density of the 1st, 2nd and 3rd trophic levels

The studies reported by Smith show the importance of the form of the model being used to determine stable densities. None of the work discussed by the author was related to actual field studies or checked to determine if actual algal populations could be predicted.

A model of algae based upon the conservation of mass has been proposed by WRE^{A-69}. This model considers three trophic levels: phytoplankton, zooplankton, and fish. Eliminating the advective mass transfer and diffusion terms, the equations are given as

$$\frac{d(VP)}{dt} = (\mu_i - r - s)\, P_i - \frac{1}{Y_z}\, g\, P_{fi}\, Z \qquad \text{(A-81)}$$

$$\frac{d(VZ)}{dt} = Z \sum_{i=1}^{2} g_i\, P_{fi} - MZ - \frac{1}{Y_f}\, \gamma F \qquad \text{(A-82)}$$

$$\frac{d(VF)}{dt} = \frac{1}{V}\, F \sum_{j=1}^{n} \gamma_j\, V_j - hF \qquad \text{(A-83)}$$

and the detritus is accounted for as

$$\frac{dD}{dt} = SP + \frac{M}{Y_z}\, Z - K_d D \qquad \text{(A-84)}$$

where

P_i = mass concentration of phytoplankton in group i

P = total mass concentration of phytoplankton

Z = mass concentration of zooplankton

D = detritus

μ_i = specific growth rate of algae

r = respiration rate

S = settling rate

Y_Z = yield coefficient of zooplankton

g = specific growth rate of zooplankton

P_{fi} = preference factor for phytoplankton in group i

M = mortality of zooplankton

γ = specific growth rate of fish

F = biomass of fish

Y_F = yield coefficient for fish

γ_j = specific growth rate of fish for element j

V_j = volume element j

V = total volume of the system

h = harvesting factor including migrating fish which leave the system

K_d = rate of bacteria degradation

This model considers two groups of phytoplankton so Equation A-81 would be written twice.

The authors propose to calculate the effect of nutrients and light on the specific growth rate for phytoplankton based on a Michaelis-Menton expression of the form

$$\mu = \hat{\mu}\left(\frac{x_1}{K_1+x_1}\right)\left(\frac{x_2}{K_2+x_2}\right) - - - \left(\frac{x_n}{K_n+x_n}\right) \qquad \text{(A-85)}$$

where

μ = specific growth rate

$\hat{\mu}$ maximum specific growth rate if all factors are in excess

K_i = Michaelis-Menton constant for factor of i

x_i = concentration or intensity of factor of i

The phytoplankton respiration rate is assumed to be constant and the settling rate is calculated by the ratio of the settling velocity of the algae to the surface overflow rate of the water. The specific growth rate for zooplankton would be calculated according to a reaction described by Smith[A-68] and given by Equation A-80.

Another model based upon the conservation of mass has been developed and tested by DiToro, et al.[A-70]. The equations for volume element V_j are

$$\dot{P} = [G_p - D_p]\ P \qquad \text{(A-86)}$$

$$\dot{Z} = [G_z - D_z]\ Z \qquad \text{(A-87)}$$

$$\dot{N} = S_n \qquad \text{(A-88)}$$

where

$$G_p = F_1\ T \left[\frac{2.718}{k_e H}\ f \left(e^{-\alpha_1} - e^{-\alpha_o} \right) \frac{N}{K_m + N} \right] \qquad \text{(A-89)}$$

$$D_p = F_2 T + C_g Z \qquad \text{(A-90)}$$

$$G_z = A_{zp}\ C_g\ K_{mp} \left(\frac{P}{K_{mp} + P} \right) \qquad \text{(A-91)}$$

$$D_z = F_3 T + F_4 \qquad \text{(A-92)}$$

$$S_n = \frac{W_n}{V} - A_{np} G_p\ P + A_{np}\ C_g\ ZP \left[1 - \frac{A_{zp}\ K_{mp}}{K_{mp} + P} \right] \qquad \text{(A-93)}$$

$$+ A_{np}\ K_2\ TP + A_{nz}\ K_3 TZ$$

in which

P = phytoplankton concentration

C_p = phytoplankton growth rate

D_p = phytoplankton death rate

Z = zooplankton concentration

G_z = zooplankton growth rate

D_z = zooplankton death rate

N = nitrate-nitrogen concentration

S_n = functional relations given above

F_1 = saturated growth rate of phytoplankton

T = temperature

f = photoperiod

k_e = extinction coefficient

H = depth

α_1 = (I_a/I_s) exp (-keH)

I_a = average incident ratiation

I_s = saturated radiation

K_m = Michaelis constant for total inorganic nitrogen

F_2 = endogenous respiration rate of phytoplankton

C_g = zooplankton grazing rate

α_o = I_a/I_s

A_{nz} = zooplankton nitrogen-carbon ratio

A_{zp} = zooplankton conversion efficiency

K_{mp} = phytoplankton Michaelis constant

F_3 = zooplankton endogenous respiration rate

F_4 = zooplankton death due to other causes

W_n = discharge rate of nitrogen

V = volume element

A_{np} = phytoplankton nitrogen-carbon ratio

This model considers two trophic levels and one limiting nutrient. If more than one nutrient is limiting, then additional Michaelis-Menton terms can be put in Equation A-89 to decrease the saturated growth rate. This model was tested in a relatively shallow reach of the San Joaquin River with reasonable success.

In both of the models discussed above the maximum growth rate for the phytoplankton was reduced by a factor based on the Michaelis-Menton equation. Shelef, et al.[A-71] have determined that a better fit to the data when nitrate is the limiting factor is obtained with an expression of the form

$$\mu = \mu_{max} \left(1-e^{S_N/K_A}\right) \qquad \text{(A-94)}$$

where

S_N = concentration of nitrate-nitrogen

K_A = constant

The constant K_A is determined empirically. An expression similar to Equation A-94 is referenced by Shelef where K_A is replaced by the Michaelis-Menton constant K_S.

The reduction in phytoplankton growth as a function of light intensity is presented by DiToro, et al.[A-70] as

$$F(I) = \frac{I}{I_S} \exp \quad 1 - \left(\frac{I}{I_S}\right) \qquad \text{(A-95)}$$

and by WRE[A-69] as

$$F(I) = \frac{I}{K_I + I} \qquad \text{(A-96)}$$

where

$F(I)$ = reduction of algae growth rate due to reduced illumination

I_S = saturated irradiance

I = irradiance

K_I = constant

Shelef, et al.[A-72] have reviewed expressions of the forms given by Equations A-95 and A-96 that were presented by other researchers. In addition, these authors note that in many cases a linear approximation is sufficient:

$$F(I) = K_I I \qquad I \leq I_S \tag{A-97}$$

and

$$F(I) = K_O \qquad I \geq I_S$$

The effects of settling of algae on the algae concentrations has been investigated by Bella[A-73], who assumed that the settling velocities of the algae are constant with time and depth and that the diffusion constant for the algae accounts for all its movement. He also assumed that the diffusion constant for algae was the same as the thermal diffusion coefficient. The data for this study were taken from Lake Sammamish, Washington. The study showed that the algae concentrations were quite sensitive to the settling velocities and that the vertical mixing had significant effect on the algae species present.

TOXIC COMPOUNDS

The behavior of toxic compounds in the aquatic environment is quite complex and in many cases unpredictable. For example, Ziebell, et al.[A-74], in a study at Port Angeles Harbor, found that levels of sulfides toxic to juvenile salmon would appear and disappear quite rapidly in localized areas throughout the harbor. The sulfides came from the anaerobic decomposition of bottom sludge deposits resulting from waste discharges from pulp and paper mills. The factors that can affect the distribution and fate of toxicants in water have been enumerated by Dawson, et al.[A-75] and are shown in Figure A-7. Very little published literature concerning modeling of toxic compounds was found in the literature survey.

One method of predicting the distribution of toxic compounds is to treat the substance as a conservative compound; i.e., to assume that the compounds are not altered by chemical or biological reactions. Hence, concentration as a function of space and time is determined solely by hydrodynamic considerations (convective transport, dispersion, and dilution). Such an approach was used by Armstrong, et al.[A-76] in a study of the toxic effects of wastes in the San Francisco Bay. The authors used two methods of transporting waste materials; one was an empirical model based on distance from the source and residence time and the other was a hydrodynamic model. Good correlation was obtained with both methods. However, it should be noted that their method considered the gross toxicity due to all wastes present and not the effect of a single toxicant.

In general most toxic compounds are not conservative and will interact with the environment. One well known example is the pesticide DDT. Eberhardt, et al.[A-77] proposed a model to describe the behavior of DDT in a freshwater marsh. They found that equations of the form

$$\frac{dy}{dt} = \lambda(t) - \mu y \qquad \text{(A-98)}$$

where

y = concentration of DDT

$\lambda(t)$ = input source of DDT

μ = rate constant

could be used to describe the movement of DDT from one part of the environment (water) to another (plants). Rate constants were determined for a number of plants and animals.

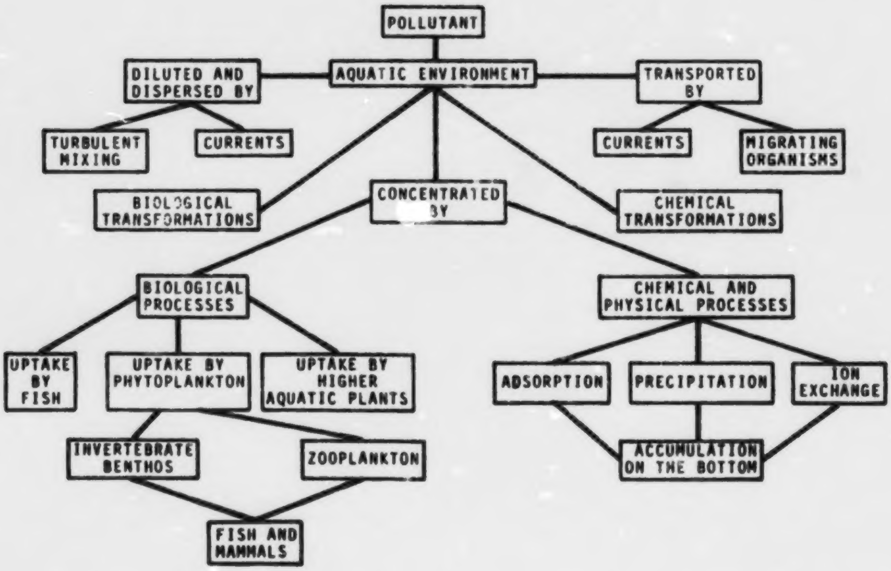
POLLUTANT
AQUATIC ENVIRONMENT
DILUTED AND DISPERSED BY
TURBULENT MIXING
CURRENTS
TRANSPORTED BY
CURRENTS
MIGRATING ORGANISMS
BIOLOGICAL TRANSFORMATIONS
CONCENTRATED BY
CHEMICAL TRANSFORMATIONS
BIOLOGICAL PROCESSES
CHEMICAL AND PHYSICAL PROCESSES
UPTAKE BY FISH
UPTAKE BY PHYTOPLANKTON
UPTAKE BY HIGHER AQUATIC PLANTS
ADSORPTION
PRECIPITATION
ION EXCHANGE
INVERTEBRATE BENTHOS
ZOOPLANKTON
ACCUMULATION ON THE BOTTOM
FISH AND MAMMALS

FIGURE A-7. FACTORS AFFECTING THE DISTRIBUTION AND FATE OF TOXICANTS IN WATER (FROM DAWSON, ET AL.[A-75])

SECTION A-2

REVIEW OF HYDRAULIC MODELS

The problem of mathematically modeling the hydraulics of most fluid systems is not, in general, a problem of formulating theoretical constructs or governing equations but rather of devising workable numerical techniques to solve established hydrodynamic or hydraulic equations. Consequently, a sound evaluation of the various models must be based on the computational aspects (i.e., stability, accuracy, solution time, etc.).

Many different concepts are involved in mathematically formulating the dynamics of fluid motion for real systems. However, the laws for conservation of mass, momentum and energy provide the primary basis for establishing comprehensive mathematical statements of the dynamics of any fluid system as a continuum. The conservation equations are:

Mass continuity

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) + \frac{\partial}{\partial z}(\rho w) = 0 \tag{A-99}$$

Momentum

$$\begin{aligned} \rho \frac{\partial u}{\partial t} + \frac{u\partial u}{\partial x} + \frac{v\partial u}{\partial y} + \frac{w\partial u}{\partial z} + 2\Omega\ (w\cdot\cos\phi - v\cdot\sin\phi) \\ = \frac{-\partial}{\partial x}(p + \gamma h) + \frac{\partial}{\partial x}\tau_{xx} + \frac{\partial}{\partial y}\tau_{yx} + \frac{\partial}{\partial z}\tau_{zx} \end{aligned} \tag{A-100}$$

$$\begin{aligned} \rho \frac{\partial v}{\partial t} + \frac{u\partial v}{\partial x} + \frac{v\partial v}{\partial y} + \frac{w\partial v}{\partial z} + 2\Omega u\cdot\sin\phi \\ = \frac{-\partial}{\partial y}(p + \gamma h) + \frac{\partial}{\partial x}\tau_{xy} + \frac{\partial}{\partial y}\tau_{yy} + \frac{\partial}{\partial z}\tau_{zy} \end{aligned} \tag{A-101}$$

$$\begin{aligned} \rho \frac{\partial w}{\partial t} + \frac{u\partial w}{\partial x} + \frac{v\partial w}{\partial y} + \frac{w\partial w}{\partial z} - 2\Omega u\cdot\cos\phi \\ = \frac{-\partial}{\partial z}(p + \gamma h) + \frac{\partial}{\partial x}\tau_{xz} + \frac{\partial}{\partial y}\tau_{yz} + \frac{\partial}{\partial z}\tau_{zz}; \text{ and} \end{aligned} \tag{A-102}$$

Energy

$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x}(uT) + \frac{\partial}{\partial y}(vT) + \frac{\partial}{\partial z}(wT) = \frac{\partial}{\partial x}\frac{(D\partial T)}{\partial x} \tag{A-103}$$

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$$\frac{\partial}{\partial y}\frac{(D\partial T)}{\partial y} + \frac{\partial}{\partial z}\frac{(D\partial T)}{\partial z} + \frac{R_T}{\rho C_\rho}; \qquad \text{(A-103)}$$

where the equations of state are given as

$\rho = \rho(T, p)$ and

$\mu = \mu(T, p)$.

The variables in the above equations are:

t = time

x, y, z = rectangular (cartesian) coordinates

$u = u(x,y,z;t)$ = velocity in x-direction

$v = v(x,y,z;t)$ = velocity in y-direction

$w = w(x,y,z;t)$ = velocity in z-direction

$p = p(x,y,z;t)$ = internal pressure

$h = h(x,y,z;t)$ = surface elevation of water

$\rho = \rho(x,y,z;t)$ = specific gravity of water

$\gamma = \gamma(x,y,z;t) = \rho g$ = specific weight of water

g = gravitational acceleration

$T = T(x,y,z;t)$ = temperature of fluid

$R_T = R_T(x,y,z;t)$ = source of sink of heat per unit, volume per unit time

c_p = specific heat of water

D = thermal diffusivity

Ω = angular velocity of the earth

Ψ = latitude

τ = shear stress tensor.

At a practical level of generalization, the above set of equations represents a general mathematical model for describing the hydraulics of any water body. However, simultaneous solution of these equations is not presently economically feasible for problems on the physical scale of an entire river basin. In actual applications of a set of judiciously chosen assumptions reduce the set of equations to forms which are specialized to particular system characterizations. Consequently, from a practical point of view the resultant set of equations can be solved numerically and provide a simplified or average description of the hydraulics in that particular system.

For mathematical modeling purposes, the hydraulic flow occurring within a river basin can be divided into three components as shown in Table A-2: 1) open channel flow; 2) tidal flow; and 3) stratified flow. Through practical assumptions, each type of flow problem can be mathematically represented as a specialized or simplified version of the general flow equations (Equations A-99 through A-103). Special numerical techniques are then applied to each hydraulic type to obtain economical and efficient solutions to the respective flow problems.

TABLE A-2. CATEGORIZATION OF THE HYDRAULIC COMPONENTS OF A RIVER BASIN SYSTEM

HYDRAULIC TYPE	RIVER BASIN COMPONENT	BASIC HYDRAULIC CHARACTERIZATION
Open Channel Flow	rivers, streams, canals and unstratified impoundments	• one-dimensional inviscid flow • hydrostatic pressure • incompressible flow
Tidal Flow	estuaries and bays	• two-dimensional inviscid flow • wind stress • geostrophic factors, such as coriolis forces, tides, etc. • incompressible flow
Stratified Flow	stratified impoundments (reservoirs and lakes)	• two-dimensional viscous flow • density stratification • wind stress

OPEN CHANNEL FLOW

Open channel flow analyses are standard and simple approaches to modeling the hydraulics of large and complex river-tributary systems, canals and aqueduct networks where a one-dimensional description is satisfactory. Such complex water systems are treated as a series of interconnected open channels and the hydraulic equations are solved to determine water depths and average velocities.

Equations of Open Channel Flow

The Saint-Venant equations approximately describe unsteady, one-dimensional, open channel flow. These equations are

Continuity

$$A \frac{\partial v}{\partial x} + \frac{v \partial A}{\partial x} + \frac{\partial A}{\partial t} = q \text{ ; and} \qquad \text{(A-106)}$$

Motion

$$\frac{\partial v}{\partial t} + \frac{v \partial v}{\partial x} = g \left(S_o - \frac{\partial h}{\partial x} - S_f\right) - \frac{qv}{A} \qquad \text{(A-107)}$$

where

A = flow area

h, v = water depth and flow velocity (average)

q = lateral inflow

g = acceleration of gravity

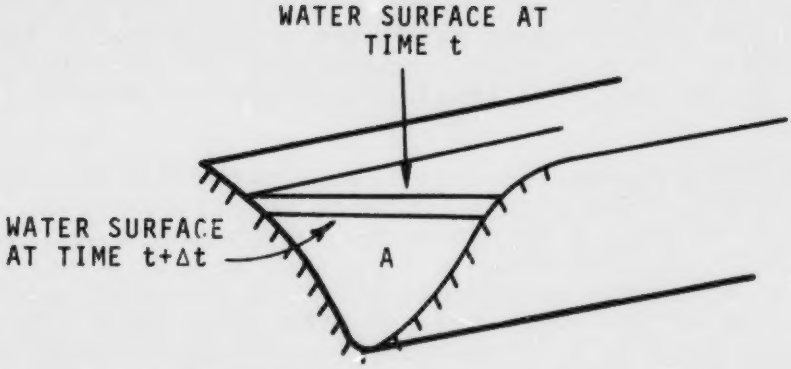
S_o, S_f = bed and friction slopes, respectively

x, t = space and time variables, respectively

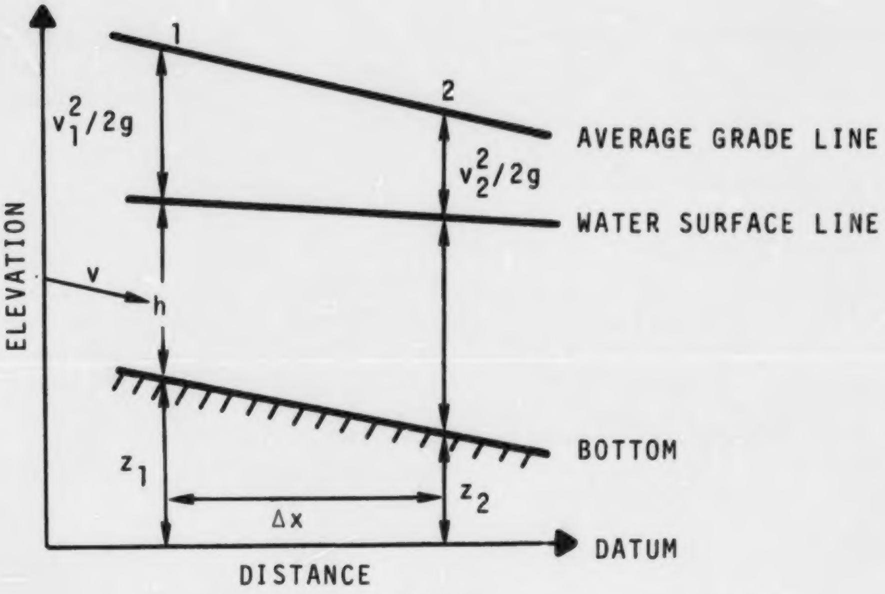
Figure A- : shows a typical open channel of arbitrary cross section.

This formulation of the Saint-Venant equations assumes:

1) gradually varying flow (no discontinuities or jumps),
2) homogeneous fluid (constant ρ),
3) unidirectional flow,
4) rigid channel, and


WATER SURFACE AT TIME t
WATER SURFACE AT TIME t+Δt
A

A-CROSS SECTIONAL AREA


1
2
$v_1^2/2g$
$v_2^2/2g$
AVERAGE GRADE LINE
WATER SURFACE LINE
ELEVATION
v
h
BOTTOM
z_1
z_2
Δx
DATUM
DISTANCE

LONGITUDINAL SECTION

FIGURE A-8. DEFINITION SKETCH FOR OPEN CHANNEL FLOW

5) channel roughness expressed by Chezy's or Manning's equation.

The derivation of these equations is given in standard texts[A-78, A-79, A-80]. The Saint-Venant equations are applicable to river basins in which river reaches, canals, and unstratified impoundments are treated as a series of interconnected channels and junctions.

Brakensiek[A-81] has observed that historically two approaches have been used for formulating general numerical solutions of unsteady open channel flow problems, the hydraulic and hydrologic methods. The hydraulic methods are based on the solution of the differential equations as expressed by the primary variables; i.e., velocity depth, area, etc. On the other hand, the hydrologic methods utilize a drastically simplified version of the momentum equation in solving the mass continuity relation in terms of volumetric flow to determine the storage profiles or flow hydrographs. The hydrologic method, although grossly approximate by theoretical standards, provides an adequate description for some types of problems. However, the hydrologic methods are inaccurate for this system of models and are not considered in this review.

In the category of hydraulic methods there are two standard numerical procedures for solving the Saint-Venant equations: direct methods and characteristic methods. Several other numerical techniques exist for formulating general solutions to open channel equations; however, almost all are variations of direct and characteristic methods.

Review of Open Channel Flow Models

Amein and Fang. Amein and Fang[A-82, A-83] report on a detailed treatment of the direct and characteristic procedures for solving the Saint-Venant Equations (A-106 and A-107). These methods of solution are applied to artificial and natural channels of the Neuse River in North Carolina. The main objective of their study was to devise, test, and compare selected versions of the fundamental numerical procedures. Specifically, three methods of solution were considered:

- implicit characteristic,
- explicit direct, and
- implicit direct.

Results of the study showed that the three methods provide almost identical solutions. However, it was concluded that the implicit direct method was more competitive and suitable for routine use. The major advantages of the implicit direct method are:

1. the method is stable for large time steps,
2. the numerical procedure is efficient and easy to program,
3. it is suitable for natural channels of complex geometry, and
4. it provides faster and more accurate computation than the implicit characteristic or explicit direct method.

Franz's[A-84] review of this work suggests that the computational advantage of the implicit direct method is only an apparent one, due mainly to the simplicity of the problem on which it was tested. Franz further indicates that numerical tests on a more complex problem would show definite increases in computation times.

Amorocho and Strelkoff. In an attempt to mathematically model the operation of the California Aqueduct, Amorocho and Strelkoff[A-85, A-86] have applied a variation of the direct explicit technique to the unsteady flow equations. The numerical sequence involves applying a change of variable to the Saint-Venant equations to make them explicit in terms of velocity and wave celerity. These equations are replaced with finite-difference analogues and solved using successive approximations.

The model describes unsteady flow in an open trapezoidal channel with a series of control structures such as gates, reservoirs, power plants, etc. The model handles channel networks and therefore would be applicable to a river network. The main limitation is the numerical inefficiency of the successive approximation solution technique and the small time step associated with explicit techniques.

Garrison, et al. The Tennessee Valley Authority has developed a river and reservoir model based on the Saint-Venant equations. Garrison, et al.,[A-87] has reported various successful applications of this particular hydraulic model to the TVA system. Calculated results obtained from calibrated versions show remarkable agreement with measured values of depth and velocity. The primary distinction of this model is that it uses an explicit numerical technique devised by Stoker[A-88]. However, like most explicit methods, this technique requires small time increments to maintain stability. In general, Garrison's report clearly demonstrates the reliability of the open channel analysis for describing the average hydraulic behavior of river systems.

Pisano. A comprehensive river basin simulation program has been developed by the FWPCA which is capable of analyzing the quality-quantity interrelationships for municipal and industrial supply, flood control, fish and aquatic life, irrigation and recreation (Pisano[A-89]).

The model by design determines probable hydrologic and water quality conditions by using kinematic routing and Monte Carlo sampling to determine the occurrence frequencies of:

1) pollutant fluxes,

2) water supply deficiencies,

3) seasonal flows, and

4) reservoir contents.

The program provides a variety of information, including statistical moments and probability distributions of:

- pollutant concentrations (at specified locations),
- reservoir levels, and
- flows.

The program requires a computer of large capacity and is limited to small networks.

WRE Hydraulic Model. Water Resources Engineers[A-90] have developed a hydrodynamic model which is applicable to estuaries, reservoirs, lakes, and rivers. The surprising versatility of the WRE model is due principally to the special application of the one-dimensional hydrodynamic equations, namely:

Momentum

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} + g\frac{\partial H}{\partial x} + K/v/v = 0 \qquad \text{(A-108)}$$

Continuity

$$\frac{\partial}{\partial x}(vA) + B\frac{\partial H}{\partial t} = 0 \qquad \text{(A-109)}$$

which in fact are the Saint-Venant equations written in terms of the primary kinetic variables (neglecting slope friction and lateral inflow terms).

The computer model requires that the physical system be represented by a network of finite elements consisting of junctions and channels. The momentum equation is applied along channels and continuity is applied at junctions. Embedded in this novel scheme is the ability to adequately describe the hydraulics of a system in one or two dimensions by using a one-dimensional equation. The computer program uses an iterative procedure to solve for flow in the component channels and for storage at junction points. In addition, the boundary conditions are such that the tide and the hydrologic input can be varied from one time interval to the next.

TIDAL FLOW

Estuaries and coastal water hydraulics are characterized by tidal influences which establish a special class of flow problem; the "long wave" nature of the hydrodynamics is a primary distinction for this case and requires a specialized analysis.

Tidal Hydrodynamics

In attempts to model tidal hydrodynamics it has been assumed that the receiving waters (estuaries, coastal seas, etc.) are well mixed unstratified bodies of water. Using the vertically integrated velocity concept introduced by Platzman[A-91], the three-dimensional hydrodynamic Equations A-99 through A-102 reduce to the following two-dimensional forms:

Continuity

$$\frac{\partial \zeta}{\partial t} + \frac{\partial (HU)}{\partial x} + \frac{\partial (HV)}{\partial y} = 0 \qquad \text{(A-110)}$$

X-momentum

$$\frac{\partial U}{\partial t} + \frac{U \partial U}{\partial x} + \frac{V \partial U}{\partial y} - FV + g \frac{\partial \zeta}{\partial x} + g \frac{U(U^2+V^2)^{1/2}}{C^2 H} - \frac{1}{\sigma H} \tau_x^s = 0 \qquad \text{(A-111)}$$

Y-momentum

$$\frac{\partial V}{\partial t} + \frac{U \partial V}{\partial x} + \frac{V \partial V}{\partial y} + FU + g \frac{\partial \zeta}{\partial y} + g \frac{V(U^2+V^2)^{1/2}}{C^2 H} - \frac{1}{\sigma H} \tau_y^s = 0 \qquad \text{(A-112)}$$

where U and V are vertically averaged velocity components of U and V as defined by

$$U = \frac{1}{H+\zeta} \int_{-h}^{\zeta} udz$$

$$V = \frac{1}{H+\zeta} \int_{-h}^{\zeta} vdz$$

where

F = Coriolis parameter

g = acceleration gravity

C = Chezy coefficient

τ_x^s = component of wind stress in x direction

τ_y^s = component of wind stress in y direction

ρ = water density

h = distance from the reference plane to the bottom

ζ = water level elevation relative to the reference plane

$H = h+\zeta$

The wind stress components are given by Dronkers[A-92,A-93] as

$$\tau_x^s = \theta_{\rho_a} W^2 \sin\psi \qquad \text{(A-113)}$$

$$\tau_y^s = \theta_{\rho_a} W^2 \cos\psi \qquad \text{(A-114)}$$

with

θ = wind stress coefficient

ρ_a = atmospheric density

W = wind velocity

ψ = angle between the wind direction and the Y-axis

Only recently have special numerical methods been devised for solving the tidal flow Equations A-110, A-111, and A-112. The primary difficulties of solving the governing equations arise from the nonlinearity of the problem, e.g., $U \partial U/\partial x$, $V \partial V/\partial y$, and the coupling of the equations through the unknowns U, V, and ζ. Actually, four numerical procedures may be applied to the problem, each with varying degrees of approximation. These methods are:

1. integral analyses,
2. linearization (perturbation methods),
3. method of characteristics, and
4. finite difference techniques.

For applications to natural physical systems (e.g., estuaries, coastal seas, or complex geometries and general boundary conditions) sophisticated finite difference schemes have been devised which are useful and efficient in studying long-term average motion and water level fluctuations induced by tidal forces.

Review of Tidal Flow Models

Leendertse. A numerical model developed by Leendertse[A-94,A-95,A-96] is based on the vertically integrated equations of motion and continuity, Equations A-110, A-111, and A-112. The model is developed specifically for tidal computations and may be applied to marine and estuarine problems of arbitrary geometry and bottom topography. The main credential for the viability of Leendertse's model lies in a multioperation finite-difference scheme which he devised specifically for the hydrodynamic equations. Leendertse has devoted a complete study to the stability of his multioperation procedure which combines implicit and explicit procedures. Results from this study show that the scheme is unconditionally stable; however, solution accuracy deteriorates for large time steps. Documented applications of the model to Tokyo Bay, Jamaica Bay, and Haringrhiet (North Sea) show favorable comparisons between observed and computed results.

Mungall and Mathews. Recent efforts at the University of Alaska to construct a complete numerical model of fjord inlets has led to the development of a general-purpose computer program for modeling tidal flow hydrodynamics. The model as reported by Mungall and Mathews[A-97] applies to variable-boundaries and the program structure is oriented toward the general user. The numerical model is based on the set of equations developed by Hansen[A-98] and Yuen[A-99], namely:

X-momentum

$$\frac{\partial U}{\partial t} + \Gamma(U^2 + V^2)1/2\,\frac{U}{H} - FV + g\,\frac{\partial z}{\partial x} = 0 \qquad \text{(A-115)}$$

Y-momentum

$$\frac{\partial v}{\partial t} + \Gamma(U^2 + V^2)1/2\,\frac{V}{H} + FU + g\,\frac{\partial z}{\partial y} = 0 \qquad \text{(A-116)}$$

Continuity

$$\frac{\partial \zeta}{\partial t} + \frac{\partial (HU)}{\partial x} + \frac{\partial (HV)}{\partial y} = 0 \qquad \text{(A-117)}$$

where

U = x - component of depth-mean velocity

V = y - component of depth-mean velocity

ζ = vertical tide measured from mean sea level

D = depth of water beneath mean sea level

H = total depth of water ($H = D + \zeta$)

Γ = friction coefficient

F = Coriolis parameter [$F = 2\Omega \sin$ (latitude)]

g = acceleration due to gravity

Ω = angular rotational speed of the earth

The equations basically neglect the nonlinear convective-inertia terms and the wind stress terms, i.e., $U\partial U/\partial x$, $V\partial U/\partial x$, $U\partial V/\partial x$, $V\partial V/\partial y$ and τ^s_x, τ^s_y, respectively.

A leap-frog numerical technique based on explicit finite-differences is used to solve the linearized equations on a space and time staggered scheme devised by Richardson[A-100].

Two applications of the model include simulations of the Gulf of California and Cook Inlet in Alaska. Tidal computations are verified for these two cases through comparisons with documented survey data (U.S.C.&G. Survey - 1968 and U.N.A.M. - 1967). The authors report adequate results although no detailed comparisons are provided.

Reid and Bodine. Reid and Bodine[A-101] developed a two-dimensional hydraulic model for simulating storm surges in Galveston Bay. This model is based on the vertically integrated equations of motion and continuity allowing for nonuniform wind effects and rainfall; however, convective inertia and Coriolis forces are ignored and the bottom friction is assumed constant. Mathematically the model is formulated as:

X-momentum

$$\frac{\partial U}{\partial t} + g\, D \frac{\partial \zeta}{\partial x} = KW^2 \cos\psi - \frac{F}{D^2}(U^2 + V^2)^{1/2} U \qquad \text{(A-118)}$$

Y-momentum

$$\frac{\partial V}{\partial t} + g\, D \frac{\partial \zeta}{\partial y} = KW^2 \sin\psi - \frac{F}{D^2}(U^2 + V^2)^{1/2} V \qquad \text{(A-119)}$$

Continuity

$$\frac{\partial \zeta}{\partial t} + \frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = R \qquad \text{(A-120)}$$

where

D = depth

K = wind stress coefficient

R = rainfall rate

F = friction coefficient

The computational model is based on a space and time staggered, explicit finite-difference scheme. Numerical stability requirements of this particular leap-frog scheme are the main limitations as small time increments must be used. The model has been calibrated and verified with observed data.

Masch, et al. Masch, et al.,[A-102,A-103] have developed a two-dimensional time-dependent numerical model for describing the tidal hydrodynamics in shallow well-mixed estuaries. The model accounts for the various physiographic features found in shallow irregularly shaped estuaries and for variable inflows, tidal action, wind stress, variable bottom friction, and coriolis forces (Equations A-118 through A-120) without rainfall.

The computational techniques of this model are based on the explicit methods used by Reid and Bodine[A-101] with modification to improve stability.

The model has been calibrated and verified with observed Galveston Bay data.

Callaway, Byram, and Ditsworth. In general, standard approaches for solving the equations of unsteady open channel flow have concentrated on the numerical analysis aspects of the problem and so individual techniques are basically variations of the methodology for numerical discretization of the equations. However, a somewhat different approach to the problem consists of applying a simple discretization of the natural system. More specifically, the physical region may be subdivided into a number of discrete segments or finite elements and the equations of flow solved for each element according to their interconnectivity. The main distinction here is that the continuity equation is solved at junctions or node points while the momentum equation is solved along element lengths.

This approach is credited to WRE and has been applied successfully to simulation of estuarial networks of the Sacramento-San Joaquin Delta and to models of the Columbia River. A general purpose computer program originally written by Water Resources Engineers was later modified, updated and refined by the Federal Water Pollution Control Administration, as reported by Callaway, Byram, and Ditsworth[A-104].

The FWPCA hydraulic model formulates the Saint-Venant equations in a more specialized form, namely:

Continuity

$$\frac{\partial}{\partial x}(vA) + B\frac{\partial H}{\partial t} = 0 \qquad \text{(A-121)}$$

Momentum

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = -g\frac{\partial H}{\partial x} + k/v/v = 0 \qquad \text{(A-122)}$$

where

v = average channel velocity during a time step (Δt)

A = cross-sectional area of channel

H = height of water surface above (arbitrary) horizontal datum

B = channel width

g = acceleration of gravity

k = friction factor

The basic assumptions are:

1. Acceleration and momentum transfer normal to the x-axis are negligible. Thus, tributary inflows contribute to a change in junction head but impart no momentum during the contribution.

2. Wave length is at least twice channel depth. If not, the shallow water assumption utilized here (in which wave celerity = $\sqrt{gh}$) would not hold. The "wave" referred to here is of tidal period, not a wind wave.

3. Coriolis and wind forces are negligible.

4. Each channel is straight (hence, no centrifugal effects) and the cross-sectional area does not vary over its length.

The slope terms in Equation A-111 have been lumped in Equation A-122 so that

$$g\left(\frac{\partial h}{\partial x} - S_o\right) = \frac{\partial H}{\partial x} \quad \text{and } S_o = 0 \qquad \text{(A-123)}$$

and the friction slope has been replaced by the Chezy equation

$$S_f = \frac{v^2}{C^2 R} \qquad \text{(A-124)}$$

It is important to note however that the Chezy equation is an empirical relationship and in fact valid only for steady flow. Thus the use of this equation in the momentum equation (A-122) is by definition an approximation.

A modified and extended version of the WRE model has been incorporated into the Storm Water Management^{A-105} program TRIUMVIRATE. This version of the model includes a wind stress term which may be important in estuary, lake and reservoir simulations. Alternate boundary conditions include 1) specified tides for estuaries, 2) weir equations for lakes and reservoirs, and 3) stage-flow relationships or inflow hydrographs (tables) for rivers. Test applications of this model have been based on engineering evaluation of the results and no comparisons with actual data have been made.

SECTION A-3

RESERVOIR MODEL LITERATURE REVIEW

STRATIFIED FLOW

In general, stratified flow in a deep reservoir may be described as fluid motion in a gravitational field which is influenced or originated by the variations in fluid density. Temperature variations are often analogous with density variations although stratification may occasionally be due to chemicals, wastes, or suspended sediments. Density variations occur frequently in nature where the mixing action induced by natural fluid motion is incomplete. Principal causes of thermal stratification in a deep reservoir are (1) limited penetration and transmission of solar radiation, (2) low thermal conductivity of water, and (3) seasonal variations in temperature of inflowing water. An annual cycle of temperature changes may be observed in most deep reservoirs. This begins in early spring with a near isothermal condition and is followed by the development of thermal stratification. Finally, in winter, upwelling occurs with a return to a near uniform thermal condition.

Equations for Stratified Flow

The inherent complexity of the problem of modeling stratified flow systems is demonstrated by the fact that all previous attempts have resorted to various simplifications. Simplifying assumptions are generally made which characterize the density variation as discrete, multi-layer, or continuous. One popular assumption is the Boussinesq approximation ($\rho = \rho_\infty(z) + \Delta\rho$) which may be used to formulate a 'reduced' set of equations describing the motion of a heterogeneous incompressible fluid, namely:

Continuity

$$\nabla \vec{V} = 0 \qquad \text{(A-125)}$$

Momentum

$$\frac{D\vec{V}}{Dt} = \nu \nabla^2 \vec{V} + (1-\beta(T-T_o))g\delta \qquad \text{(A-126)}$$

Energy

$$\frac{DT}{Dt} = \frac{K}{\rho c_p} \nabla^2 T + \frac{q}{\rho c_p} \qquad \text{(A-127)}$$

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where

$\vec{V}$ = velocity vector

ν = kinematic viscosity

β = thermal coefficient of volumetric expansion

T = temperature

T_o = reference temperature

g = acceleration of gravity

δ = Kronecker delta (Z component $\delta_z = 1$, otherwise $\delta_x = \delta_y = 0$)

$K/\rho c_p$ = thermal diffusivity

q = volumetric heat generation

ρ = density

c_p = heat capacity

Other assumptions are implicit in the above formulation:

1. diffusivity, viscosity, density, thermal conductivity, and heat capacity are constant;
2. dynamic pressure is negligible; and
3. there are no variations in density due to chemical changes.

The reduced set of governing equations with an appropriate set of initial and boundary conditions constitutes a general model which can adequately describe the hydrodynamics in reservoirs, impoundments, and some lakes.

Review of Reservoir Models

Slotta, L., et al. Larry Slotta, et al.[A-106] presents the NUMAC method for solving a 'specialized' set of equations which describe the transient flow of a nonhomogeneous, viscous, incompressible fluid. Slotta's model formulation is based on a layered characterization of the stratification. The stratified flow model is expressed by:

Continuity

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \qquad \text{(A-128)}$$

Incompressibility

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + v\frac{\partial \rho}{\partial y} = 0 \qquad \text{(A-129)}$$

x-Momentum

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2) + \frac{\partial}{\partial y}(\rho uv) = \rho g_x - \frac{\partial p}{\partial x} + 2\frac{\partial}{\partial x}(\mu\frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(\mu\frac{\partial u}{\partial y}) + \frac{\partial}{\partial y}\mu(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}) \qquad \text{(A-130)}$$

y-Momentum

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho uv) + \frac{\partial}{\partial y}(\rho v^2) = \rho g_y - \frac{\partial P}{\partial y} + 2\frac{\partial}{\partial x}(\mu\frac{\partial v}{\partial x}) + \frac{\partial}{\partial y}(\mu\frac{\partial v}{\partial y}) + \frac{\partial}{\partial x}\mu(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}) \qquad \text{(A-131)}$$

where

ρ = density

u, v = velocity components

g_x, g_y = gravitational components

μ = viscosity

P = pressure

This specialized formulation of the governing equations eliminates the task of solving the heat equation and equation of state, which are required in the classical formulation. The set of governing equations and an appropriate set of initial and boundary conditions constitutes a general two-dimensional model for thermally stratified flow systems, e.g., impoundments, reservoirs, and lakes.

NUMAC, a method for Nonhomogeneous Unconfined Marker-And-Cell calculation, is basically an extension of the Marker-And-Cell (MAC) method developed by Welch, et al.[A-107]. The main distinction of the NUMAC method is that it was devised specifically for two types of nonhomogeneities, intrusions of one fluid into another (miscible displacement) and density stratified flows; however, there is no restriction to these types of density variations. The NUMAC algorithm uses a combined Eulerian-Lagrangian system on which it solves finite-difference representations of the governing equations iteratively. In the scheme, the velocity and pressure are considered as Eulerian variables (i.e., defined on a fixed grid network) while density is a Lagrangian variable.

The primary limitation of this method is its implementation. For example, (1) it treats rectangularized boundaries only, (2) it requires very large run times (stability requirements establish time step size), (3) the computer program requires large computer storage (65,000 locations), and (4) detail is limited to small grid networks (e.g., 800 cells).

Despite the present limitations on the use of the NUMAC method the authors have demonstrated its usefulness in solving problems of current engineering interest such as flow into a stratified tank, wave motion over a submerged conduit, withdrawal from a density stratified reservoir, and others.

A detailed description of the numerical technique is not included here due to the lengthy and complex nature of the mathematics.

Liggett. Liggett[A-108,A-109,A-110,A-111] has addressed the important problem of modeling circulation currents in stratified lakes. This particular problem has practical applications to storage waters where stratification predominantly affects water quality, as in reservoirs and impoundments.

Based on a two-layer characterization of stratification, the hydrodynamic equations for each layer are formulated in three dimensions as:

x-Momentum

$$-fv = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \eta\frac{\partial^2 u}{\partial z^2} \qquad \text{(A-132)}$$

y-Momentum

$$fu = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \eta\frac{\partial^2 v}{\partial z^2} \qquad \text{(A-133)}$$

z-Momentum

$$g = -\frac{1}{\rho}\frac{\partial p}{\partial z} \qquad \text{(A-134)}$$

Continuity

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \qquad \text{(A-135)}$$

where

x, y, z = spatial coordinates

u, v, w = velocity components along x, y, z, respectively

ρ = density

p = pressure

η = eddy viscosity

g = acceleration of gravity

With appropriate boundary and interface conditions, the "linearized" hydrodynamic equations are solved by a combined "analytical-numerical" approach. Specifically, for each layer Equations A-132, A-133 and A-134 are solved analytically while the continuity equation is solved numerically via a stream function approach. The set of governing equations are solved iteratively for each layer until the solutions are continuous at the interface.

Liggett's model is able to generate steady-state point velocities, pressures, and thermocline locations for lakes of arbitrary plan, form, and bottom topography. However, due to certain numerical difficulties the model has had only limited use and no field verification to date.

Water Resources Engineers, Inc. WRE[A-112,A-113] has approached the complex problem of thermally stratified flow with a very rudimentary diffusion and buoyancy analysis which has established a novel pattern for a generation of reservoir simulation models. A model structure is developed around a simplified segment-layer discretization of the actual reservoir geometry. Heat and mass inventories for the discrete layers are used to formulate the basic structure of the math model. The basic heat budget is expressed as:

Heat Budget

$$\frac{dH}{dt} = h_{sw} + h_i - h_o - \left\{ h_v\Big|_{z+\Delta z} - h_v\Big|_{z} \right\} - \left\{ h_d\Big|_{z+\Delta z} - h_d\Big|_{z} \right\} \qquad \text{(A-136)}$$

where

H = heat stored in a control volume of thickness Δz

h_i = heat advected to control volume by fluid inflow

h_o = heat advected from control volume by fluid outflow

h_{sw} = heat flow by direct short-wave insolation

h_v = heat flow by advection along the vertical axis

h_d = heat flow by diffusion along the vertical axis

t = time

This heat budget is expressed for a discrete layer or element as:

Heat Equation

$$\begin{aligned} \frac{a_{j+1}+a_j}{2}\frac{d\theta_j}{dt} &= \frac{a_{j+1}+a_j}{2}\frac{h'_j}{c\rho} + \frac{1}{\Delta z}\left\{ Q_{i_j}\theta_i - Q_{o_j}\theta_j \right\} \\ &\quad - \frac{1}{\Delta z}\left\{ Q_{vo_j}\theta_j - Q_{vi_j}\theta_{j-1} \right\} + \frac{a_{j+1}A_{j+1}}{\Delta z^2}\theta_{j+1} \qquad \text{(A-137)} \\ &\quad - \frac{a_{j+1}A_{j+1}+a_jA_j}{\Delta z^2}\theta_j + \frac{a_jA_j}{\Delta z^2}\theta_{j-1} \end{aligned}$$

where

c = heat capacity of water

ρ = density of water

a_{j+1} = area of upper plane bounding the jth element

a_j = area of lower plane bounding the jth element

h'_j = change in external solar heat flux per unit of water depth

A_{j+1} = coefficient of "effective" diffusivity at the upper boundary of the jth element

A_j = coefficient of "effective" diffusivity at the lower boundary of the jth element

θ_j = temperature

Q_{vo} = vertical flow rate out of the element

Q_{vi} = vertical flow rate into the element

Q_i = horizontal inflow into the element

Q_o = horizontal outflow from the element

Similarly, the water budget for an element is formulated as:

Continuity

$$Q_{vi_j} = \sum_{k=1}^{j-1} (Q_{i_k} - Q_{o_k}) \qquad \text{(A-138)}$$

In conjunction with these gross heat and water balances a highly simplified rationale is employed to account for the hydrodynamics of the problem. Buoyancy effects are assumed to dominate the inertial contributions, which are ignored; based on this assumption, flows are routed into segment-element geometries according to density compatibility. Within the zone of withdrawal an empirical analysis is used to estimate the thickness of a withdrawal layer. A flow distribution is as assumed for this region. For multiple withdrawals, the assumed flow profiles are superimposed to obtain the estimated horizontal flow profiles.

A number of restrictive properties in this type of model are intrinsic to the kind of analysis used. However, several documented field applications[A-112,A-113] of this model appear to satisfy most critical scrutiny; its ability to predict temperature patterns is generally adequate.

Currently there are at least two or perhaps three versions of this model in use. They are distinct principally in that they are single segment versions of multi-segment programs.

Clay and Fruh.[A-114] Clay and Fruh's model is very similar to the WRE model, containing segment-element discretization, one-dimensional heat equation, gross water balance, and analytical-empirical formulation. There are four main components to the math model:

1. prediction of impoundment heat exchange and diffusion;
2. description of reservoir withdrawal hydraulics;
3. accounting for continuous changes in heat and water budgets; and
4. prediction of water quality (conservative substances only) in terms of inflows.

Clay's approach varies from that of WRE in that his simplifying assumptions are generally consistent with the complexity of his model.

A simple interaction is assumed to occur between the net external heat exchange at the air-water interface and the internal heat exchange; the external heat exchange is assumed to occur within the top layer only.

The internal heat exchange is formulated simply as:

Heat Budget

$$\frac{\partial Q}{\partial t} = -E_z \frac{\partial T}{\partial z}\, dxdy \qquad \text{(A-139)}$$

where

$\frac{\partial Q}{\partial t}$ = heat flux enter a control volume

E_z = effective diffusion coefficients

$\frac{\partial T}{\partial z}$ = vertical temperature gradient

dx, dy = spatial increment in x and y.

From this Fickian formulation of the heat flux, a difference approximation in terms of temperature may be derived for an elemental layer.

Heat Equation

$$T_i^{(k+1)} = T_i^{(k)} + \frac{E_{z_i}}{2\rho c}\,\frac{\Delta t}{\Delta z^2}\left[T_{i+1}^{(k)} - T_{i-1}^{(k)}\right] \qquad \text{(A-140)}$$

where

$T^{(k)}$, $T_i^{(k+1)}$ = temperatures for the i^{th} layer at the k and k+1 time planes

ρ = density

c = specific heat

Effective diffusion is assumed to decrease logarithmically from the water surface.

The hydraulics of stratified flow are lumped into density compatibility arguments and analytical-empirical solutions, e.g., Koh's solution and the Bohan-Grace solution for the distribution of flows near a withdrawal zone.

The model verification was conducted at Lake Travis in Texas, with numerous comparisons of temperature and chemical quality predictions. The predicted temperature patterns, temperature histories (total heat content), and quality histories were compared with observed data and in each case the results were highly encouraging.

Ryan, P. J., and D. R. F. Harleman. A reservoir model originally developed by Huber and Harleman[A-115] has been modified, refined, and well-documented by Ryan and Harleman[A-116]. This comprehensive reservoir model was based on the popular segment-layer discretization and considers (1) adsorption and transmission of solar radiation, (2) convection due to surface cooling, (3) boundary heat sources and sinks, (4) heat transport by advection and diffusion, and (5) a buoyancy rationale, i.e., no inertia, for routing inflows according to density compatibility.

The basic heat equation is derived for a layer as:

Heat Equation

$$\frac{\partial T}{\partial t} = \frac{\alpha}{A} \frac{\partial}{\partial z} \left(A \frac{\partial T}{\partial z}\right) - \frac{1}{\rho c A} \frac{\partial}{\partial z} (A\phi) - \frac{1}{A} \frac{\partial}{\partial z} (vAT) + \frac{1}{A} (u_i B T_i - u_o B T) \qquad \text{(A-141)}$$

where

T = temperature at elevation z

T_i = inflow temperature

v = vertical velocity at elevation z

u_i, u_o = horizontal inflow and outflow velocities

A = area at elevation z

α = molecular diffusivity

B = width of reservoir at elevation z

By requiring that mass conservation be satisfied in the j^{th} layer, the continuity equation is expressed as:

Continuity Equation

$$v_{j+1}' = \frac{1}{\bar{A}_j} (v_j A_j + B_j \Delta z (u_{i_j} - u_{o_j})) \qquad \text{(A-142)}$$

where

Δz = thickness of the j^{th} layer

$\bar{A}_j$ = area at the midplane of the j^{th} layer

All other variables are the same as previously defined.

Gaussian profiles are assumed for the inflow and outflow velocity distributions while the thickness of the withdrawal layer is computed according to the Koh or Koa analytical solution.

Basic features of the numerical model include provisions for (1) simultaneous or intermittent withdrawal from multilevel outlets, (2) time-lag options for proper accounting for the inflow time of travel, (3) entrance mixing, (4) wind mixing, and (5) convective mixing for unstable profiles. Energy checks are performed in the program to detect and signal any large errors which might occur in the overall energy balance.

This model has been verified at Fontana Reservoir and very good agreement between predicted and measured values for outflow temperature and temperature profiles has been observed.

Markofsky, M., and D. R. F. Harleman Markofsky and Harleman[A-116] have incorporated a one-dimensional water quality model into a stratified reservoir model originally developed by Huber and Harleman[A-115] and reported by Ryan and Harleman[A-115]. The water quality model is designed to predict the quality of the outflow water as a function of time. The outflow water is assumed to come from the withdrawal layer, the vertical thickness of which is a function of the degree of thermal stratification.

The water quality model is formulated for the segment-layer discretization and considers dissolved oxygen and biochemical oxygen demand. Diffusion effects are neglected in the governing equations which are expressed as:

Quality Model

$$\frac{\partial C^{(1)}}{\partial t} + v\frac{\partial C^{(1)}}{\partial z} = -KC^{(2)} + (u_i C_i^{(1)} - u_o C^{(1)})\frac{B(z)}{A(z)} \quad \text{(A-143)}$$

$$\frac{\partial C^{(2)}}{\partial t} + v\frac{\partial C^{(2)}}{\partial z} = -KC^{(2)} + (u_i C_i^{(2)} - u_o C^{(2)})\frac{B(z)}{A(z)} \quad \text{(A-144)}$$

where

$C^{(1)}$ = dissolved oxygen (DO)

$C^{(2)}$ = biochemical oxygen demand (BOD)

K = BOD decay rate constant

u_i, u_o = horizontal inflow and outflow velocities

v = vertical velocity

$B(z)$ = width of the layer at elevation z

$A(z)$ = horizontal surface area of the layer at elevation z

The model has been tested against laboratory experiments with pulse injections of conservative tracers and time varying inflows and outflows. Good agreements have been obtained between measured and predicted concentration values. However, field applications at Fontana Reservoir showed limited success in predicting dissolved oxygen profiles; poor results may be attributed to the lack of BOD data in this particular application.

APPENDIX A

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